

Lattice QCD and Nuclear Physics

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*Lectures at the Summer School on
“Modern perspectives in lattice QCD”
Les Houches, August 3–28, 2009*

Preface

This short lecture is consist of three parts.

In the first part, the Lüscher's formula, which relates the scattering phase shift to the two particle energy in the finite volume, explained. A comprehensive but less rigorous derivation for the formula has been attempted in this lecture for the $\pi\pi$ system as an example with the emphasis on the Bethe-Salpeter(BS) wave function. It is important to note that the BS wave function at large separation behaves as the free scattering wave with the phase shift which is determined by the unitarity of the S -matrix in QCD. The Lüscher's formula can be obtained from this asymptotic behavior of the BS wave function.

In the second part, the BS wave function is considered at non-asymptotic region where the interaction between two particles exists, in order to define the potential in quantum field theories. This method is applied to the two-nucleon system in order to extract the NN potential from lattice QCD.

In the last part, the origin of the strong repulsion at short distance in the NN potential, called the repulsive core, is theoretically investigated by the Operator Product Expansion and the renormalization group.

Acknowledgements

I would like to thank the organizer of this Les Houches school for giving me an opportunity for this lecture at the school and all attendees of the school for stimulating discussions. I also thank members of HAL QCD(Hadron to Atomic nuclei from Lattice QCD) Collaboration, T. Doi, T. Hatsuda, Y. Ikeda T. Inoue, N. Ishii, K. Murano, K. Nemura and K. Sasaki, for providing me the latest data and useful discussions, and my collaborators and friends, J. Balog, N. Ishizuka, W. Weise and P. Weisz, for valuable discussions and comments. This work is supported in part by Grant-in-Aid of the Japanese Ministry of Education, Sciences and Technology, Sports and Culture (Nos. 20340047) and by Grant-in-Aid for Scientific Research on Innovative Areas(No. 2004: 20105001, 20105003).

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1

Introduction: Nuclear Forces

In 1935 Yukawa introduced virtual particles, pions, to explain the nuclear force (Yukawa, 1935), which binds protons and neutrons inside nuclei. Since then, enormous efforts have been devoted to understand the nucleon-nucleon (NN) interaction at low energies both from theoretical and experimental points of view. To describe the elastic nucleon-nucleon (NN) scattering at low-energies below the pion production threshold together with the deuteron properties, the notion of the NN potential turns out to be very useful (Taketani *et al.*, 1967; Hoshizaki *et al.*, 1968; Brown and Jackson, 1976; Machleidt, 1989; Machleidt and Slaus, 2001): it can be determined phenomenologically to reproduce the scattering phase shifts and bound state properties. Once the potential is determined, it can be used to study systems with more than 2 nucleons by using various many-body techniques.

Phenomenological NN potentials which can fit the NN data precisely (e.g. more than 2000 data points with $\chi^2/\text{dof} \simeq 1$) at $T_{\text{lab}} < 300$ MeV are called the high-precision NN potentials. Those in the coordinate space, some of which are shown in Fig.1.1, are known to reflect some characteristic features of the NN interaction at different length scales (Taketani *et al.*, 1967; Hoshizaki *et al.*, 1968; Brown and Jackson, 1976; Machleidt, 1989; Machleidt and Slaus, 2001):

- (i) The long range part of the nuclear force (the relative distance $r > 2$ fm) is dominated by the one-pion exchange introduced by Yukawa (Yukawa, 1935). Because of the pion's Nambu-Goldstone character, it couples to the spin-isospin density of the nucleon and hence leads to a strong spin-isospin dependent force, namely the tensor force.
- (ii) The medium range part ($1 \text{ fm} < r < 2 \text{ fm}$) receives significant contributions from the exchange of two-pions ($\pi\pi$) and heavy mesons (ρ , ω , and σ). In particular, the spin-isospin independent attraction of about 50 – 100 MeV in this region plays an essential role for the binding of atomic nuclei.
- (iii) The short range part ($r < 1 \text{ fm}$) is best described by a strong repulsive core as originally introduced by Jastrow (Jastrow, 1951). Such a short range repulsion is important for the stability of atomic nuclei against collapse, for determining the maximum mass of neutron stars, and for igniting the Type II supernova explosions (Tamagaki *et al.*, 1993; Heiselberg and V. Pandharipande, 2000; Lattimer and Prakash, 2000).

A repulsive core surrounded by an attractive well is in fact a common feature of the “effective” potential between composite particles. The Lenard-Jones potential between neutral atoms or molecules is a well-known example in atomic physics. The potential

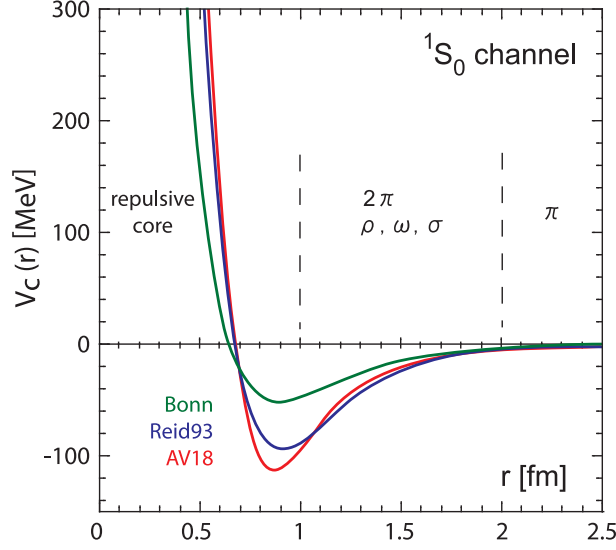


Fig. 1.1 Three examples of the modern NN potential in 1S_0 (spin singlet and S -wave) channel: CD-Bonn(Machleidt, 2001), Reid93(Stoks *et al.*, 1994) and Argonne v_{18} (Wiringa *et al.*, 1995).

between ^4He nuclei is a typical example in nuclear physics. The origin of the repulsive cores in these examples is known to be the Pauli exclusion among electrons or among nucleons. The same idea, however, is not directly applicable to the NN potential, because the quark has not only spin and flavor but also color which allows six quarks to occupy the same state without violating the Pauli principle. Therefore, to account for the repulsive core of the NN force, various ideas have been proposed as summarized in Ref. (Myhrer and Wroldsen, 1988; Oka *et al.*, 2000; Fujiwara *et al.*, 2007): exchange of the neutral ω meson (Nambu, 1957), exchange of non-linear pion field (Jackson and Pasquier, 1985; Yabu and Ando, 1985), and a combination of the Pauli principle with the one-gluon-exchange between quarks (Otsuki *et al.*, 1965; Machida and M. Namiki, 1965; Neudachin *et al.*, 1977; Liberman, 1977; DeTar, 1979; Oka and Yazaki, 1980; Oka and Yazaki, 1981*a*; Oka and Yazaki, 1981*b*; Toki, 1980; Faessler *et al.*, 1982). Despite all these efforts, convincing account of the nuclear force has not yet been obtained.

In this situation, it is highly desirable to study the NN interactions from the first principle lattice QCD simulations. A theoretical framework suitable for such purpose was first proposed by Lüscher (Lüscher, 1991): For two hadrons in a finite box with the size $L \times L \times L$ in periodic boundary conditions, an exact relation between the energy spectra in the box and the elastic scattering phase shift at these energies was derived: If the range of the hadron interaction R is sufficiently smaller than the size of the box $R < L/2$, the behavior of the two-particle Bethe-Salpeter (BS) wave function $\psi(\mathbf{r})$ in the interval $R < |\mathbf{r}| < L/2$ under the periodic boundary conditions

has sufficient information to relate the phase shift and the two-particle spectrum. Lüscher's method bypasses the difficulty to treat the real-time scattering process on the Euclidean lattice. Furthermore, it utilizes the finiteness of the lattice box effectively to extract the information of the on-shell scattering matrix and the phase shift.

Recently, a closely related but an alternative approach to the NN interactions from lattice QCD has been proposed (Ishii *et al.*, 2007; Aoki *et al.*, 2008; Aoki *et al.*, 2010b). The starting point is the same BS wave function $\psi(\mathbf{r})$ as discussed in Ref. (Lüscher, 1991). Instead of looking at the wave function outside the range of the interaction, the authors consider the internal region $|\mathbf{r}| < R$ and define the energy-independent non-local potential $U(\mathbf{r}, \mathbf{r}')$ from $\psi(\mathbf{r})$ so that it obeys the Schrödinger type equation in a finite box. Since $U(\mathbf{r}, \mathbf{r}')$ for strong interaction is localized in its spatial coordinates due to confinement of quarks and gluons, the potential receives finite volume effect only weakly in a large box. Therefore, once U is determined and is appropriately extrapolated to $L \rightarrow \infty$, one may simply use the Schrödinger equation in the infinite space to calculate the scattering phase shifts and bound state spectra to compare with experimental data. Further advantage of utilizing the potential is that it would be a smooth function of the quark masses so that it is relatively easy to handle on the lattice. This is in sharp contrast to the scattering length which shows a singular behavior around the quark mass corresponding to the formation of the NN bound state.

In this lecture, we first introduce the Lüscher's method for the scattering phase shift in Sec.2. Since the method is not only well established but also well explained in Ref.(Lüscher, 1991), we mainly consider properties of the BS wave function, in terms of which the scattering phase shift can be related to the energy shift of the 2 particles state in the finite box. These properties are also used to define the NN potential in Sec.3, where new method in Ref.(Ishii *et al.*, 2007; Aoki *et al.*, 2008; Aoki *et al.*, 2010b) is explained in detail. We finally consider a very recent attempt to understand the origin of the repulsive core in the NN potential in Sec.4. Using the operator product expansion and the renormalization group analysis in QCD, the potential derived from the BS wave function in Sec.3 is shown to have the repulsive core, whose functional form is also theoretically predicted(?). Brief concluding remarks are given in Sec.5.

2

Phase Shift from Lattice QCD: Lüscher's formula in the finite volume

2.0.1 Preparation: Scattering phase shift in quantum mechanics

In this subsection, as a preparation for the latter sections, we give some basics of the scattering theory in quantum mechanics.

Let us consider the 3-dimensional Schrödinger equation, given by

$$[H_0 + V(\mathbf{r})]\varphi(\mathbf{r}) = E\varphi(\mathbf{r}) \quad (2.1)$$

where

$$H_0 = -\frac{\nabla^2}{2m}, \quad \nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2. \quad (2.2)$$

Hereafter we consider only the spherically symmetric potential that $V(\mathbf{r}) = V(r)$ with $r = |\mathbf{r}|$. In this case it is convenient to use the polar coordinate such that

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{\hat{L}^2}{r^2}, \quad \hat{L}^2 = - \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]. \quad (2.3)$$

Using the separation of the variables, we consider the following form of the solution $\varphi(\mathbf{r})$:

$$\varphi(\mathbf{r}) = \sum_l R_l(r) Y_{lm}(\theta, \phi) \quad (2.4)$$

where the spherical harmonic function Y_{lm} satisfies

$$\hat{L}^2 Y_{lm}(\theta, \phi) = l(l+1) Y_{lm}(\theta, \phi) \quad (2.5)$$

$$\hat{L}_z Y_{lm}(\theta, \phi) = m Y_{lm}(\theta, \phi) \quad (2.6)$$

and is normalized as

$$\int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \overline{Y_{lm}(\theta, \phi)} Y_{l'm'}(\theta, \phi) = \delta_{ll'} \delta_{mm'}. \quad (2.7)$$

Note that in this lecture \overline{X} means a complex conjugate of X while X^\dagger is a hermitian conjugate of X . Explicitly it is given by

$$Y_{lm}(\theta, \phi) = c \sqrt{\frac{2l+1}{4\pi} \cdot \frac{(l-|m|)!}{(l+|m|)!}} P_{lm}(\cos \theta) e^{im\phi}, \quad (2.8)$$

$$c = \begin{cases} (-1)^m & m > 0 \\ 1 & m \leq 0 \end{cases} \quad (2.9)$$

where $P_{lm}(z)$ is the Legendre bi-function of degree l , defined by

$$P_{lm}(z) = (1 - z^2)^{m/2} \frac{d^{|m|} P_l(z)}{dz^{|m|}}, \quad |m| \leq l, \quad (2.10)$$

$$P_l(z) = \frac{1}{2^l l!} \frac{d^l}{dz^l} (z^2 - 1)^l. \quad (2.11)$$

For small l and m , for example, we have

$$\begin{aligned} Y_{00}(\theta, \phi) &= \frac{1}{\sqrt{4\pi}}, \quad Y_{10}(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y_{1\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}, \\ Y_{20}(\theta, \phi) &= \sqrt{\frac{5}{4\pi}} \frac{1}{2} (3 \cos^2 \theta - 1), \quad Y_{2\pm 1}(\theta, \phi) = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi}, \\ Y_{2,\pm 2}(\theta, \phi) &= \mp \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm i2\phi}. \end{aligned} \quad (2.12)$$

From eqs. (2.4) and (2.5), the 3-dimensional Schrödinger equation (2.1) is reduced to the 1 dimensional equation for R_l as

$$\frac{1}{r} \frac{d^2}{dr^2} (r R_l(r)) + \left\{ 2m(E - V(r)) - \frac{l(l+1)}{r^2} \right\} R_l(r) = 0. \quad (2.13)$$

Usually we further assume the following properties for the potential $V(r)$:

$$\lim_{r \rightarrow 0} r^2 V(r) = 0, \quad (2.14)$$

$$\lim_{r \rightarrow \infty} r^n V(r) = 0 \quad \text{for } \forall n \in \mathbf{Z}. \quad (2.15)$$

The first condition means

$$V(r) < O\left(\frac{1}{r^2}\right) \quad (2.16)$$

for small r , which leads to

$$R_l(r) = O(r^l) \quad (2.17)$$

for small r . The second condition means

$$V(r) = 0 \quad \text{for } r > R, \quad (2.18)$$

for sufficiently large R , so that eq. (2.13) becomes

$$R_l''(y) + \frac{2}{y} R_l'(y) + \left\{ 1 - \frac{l(l+1)}{y^2} \right\} R_l(y) = 0 \quad (2.19)$$

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for $r > R$, where $y = kr$ and $k^2 = 2mE$. The solution to this equation is obtained as

$$R_l(y) = A_l j_l(y) + B_l n_l(y) \quad (2.20)$$

where spherical Bessel functions are given by

$$j_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \left(\frac{\sin x}{x} \right) \simeq \begin{cases} \frac{x^l}{(2l+1)!!}, & x \rightarrow 0 \\ \frac{\sin(x - l\pi/2)}{x}, & x \rightarrow \infty \end{cases}, \quad (2.21)$$

$$n_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \left(\frac{\cos x}{x} \right) \simeq \begin{cases} \frac{x^{-(l+1)}}{(2l-1)!!}, & x \rightarrow 0 \\ \frac{\cos(x - l\pi/2)}{x}, & x \rightarrow \infty \end{cases}. \quad (2.22)$$

Therefore, in $r \rightarrow \infty$ limit, the above solution becomes

$$R_l(r) \simeq A_l \frac{\sin(kr - \frac{l}{2}\pi)}{kr} + B_l \frac{\cos(kr - \frac{l}{2}\pi)}{kr} = C_l \frac{\sin(kr - \frac{l}{2}\pi + \delta_l(k))}{kr} \quad (2.23)$$

where the scattering phase shift $\delta_l(k)$ is given by

$$\tan \delta_l(k) = \frac{B_l}{A_l}, \quad C_l = \sqrt{A_l^2 + B_l^2} \quad (2.24)$$

and $A_l = C_l \cos \delta_l(k)$, $B_l = C_l \sin \delta_l(k)$. If $\delta_l(k) > 0$ the interaction is attractive for this k , while it is repulsive if $\delta_l(k) < 0$.

For the particle-particle scattering in quantum mechanics, we consider the Lagrangean,

$$L = \frac{1}{2} m_1 \dot{\mathbf{r}}_1^2 + \frac{1}{2} m_2 \dot{\mathbf{r}}_2^2 - V(|\mathbf{r}_1 - \mathbf{r}_2|). \quad (2.25)$$

By introducing the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center of gravity $\mathbf{R} = (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2)/(m_1 + m_2)$, the above Lagrangean becomes

$$L = \frac{1}{2} M \dot{\mathbf{R}}^2 + \frac{1}{2} \mu \dot{\mathbf{r}}^2 - V(r), \quad (2.26)$$

where $M = m_1 + m_2$ is the total mass and $\mu = m_1 m_2 / (m_1 + m_2)$ is the reduced mass. The corresponding Hamiltonian is given by

$$H = H_G + H_{\text{rel}}, \quad H_G = \frac{1}{2M} \mathbf{P}^2, \quad H_{\text{rel}} = \frac{1}{2\mu} \mathbf{p}^2 + V(r), \quad (2.27)$$

where $\mathbf{P} = M \dot{\mathbf{R}}$ and $\mathbf{p} = \mu \dot{\mathbf{r}}$. While H_G is a Hamiltonian for a free particle, H_{rel} corresponds to the Hamiltonian for a particle under the potential $V(r)$, whose Schrödinger equation identical to eq.(2.1).

2.1 Bethe-Salpeter wave function and phase shift in quantum field theories

In this section, we construct a "scattering wave" in quantum field theories whose asymptotic behavior is identical to the one in the scattering wave in quantum mechanics given in eq.(2.23). Moreover we show that the phase shift corresponds to the phase of the S -matrix required by the unitarity. For notational simplicity we consider the $\pi\pi$ scattering in QCD here.

The unitarity of the S -matrix $S^\dagger S = SS^\dagger = \mathbf{1}$ with $S = 1 + iT$ leads to

$$\langle f|T|i\rangle - \langle f|T^\dagger|i\rangle = i \sum_n \langle f|T^\dagger|n\rangle \langle n|T|i\rangle, \quad (2.28)$$

where $|n\rangle$ are asymptotic states. In the case of $\pi\pi$ scattering in the center of mass system that $k_a + k_b \rightarrow k_c + k_d$ where $k_a = (E_k, \mathbf{k})$, $k_b = (E_k, -\mathbf{k})$ and $k_c = (E_p, \mathbf{p})$, $k_d = (E_p, -\mathbf{p})$ with $E_k = \sqrt{\mathbf{k}^2 + m_\pi^2}$ and $E_p = \sqrt{\mathbf{p}^2 + m_\pi^2}$, we explicitly write

$$\langle k_c, k_d|T|k_a, k_b\rangle = (2\pi)^4 \delta^{(4)}(k_a + k_b - k_c - k_d) T(\mathbf{p}, \mathbf{q}) \quad (2.29)$$

We consider the elastic scattering, where the total energy is below the 4π production such that $2\sqrt{k^2 + m_\pi^2} < 4m_\pi$, equivalently, $k^2 < 3m_\pi^2$ with $k = |\mathbf{k}| = |\mathbf{p}|$. In this case, due to the energy-momentum conservation, the sum over intermediate state n in Eq. (2.28) is restricted to the $\pi\pi$ states as

$$\sum_n |n\rangle \langle n| = \int \frac{d^3 \mathbf{p}_1}{(2\pi)^3 E_{p_1}} \frac{d^3 \mathbf{p}_2}{(2\pi)^3 E_{p_2}} |p_1, p_2\rangle \langle p_1, p_2|. \quad (2.30)$$

Inserting this into Eq. (2.28), we have

$$T(\mathbf{p}, \mathbf{k}) - T^\dagger(\mathbf{p}, \mathbf{k}) = i \frac{k}{32\pi^2 E_k} \int d\Omega_{\mathbf{q}} T^\dagger(\mathbf{p}, \mathbf{q}) T(\mathbf{q}, \mathbf{k}), \quad (2.31)$$

where $|\mathbf{q}| = k$ and $\Omega_{\mathbf{q}}$ is the solid angle of the vector \mathbf{q} . Using the partial wave decomposition that

$$T(\mathbf{p}, \mathbf{k}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l T_l(k) Y_{lm}(\Omega_{\mathbf{p}}) \overline{Y_{lm}(\Omega_{\mathbf{k}})} \quad (2.32)$$

and the orthogonal property of the spherical harmonics function $Y_{lm}(\theta, \phi) = Y_{lm}(\Omega_{\mathbf{q}})$ that

$$\int d\Omega_{\mathbf{q}} \overline{Y_{lm}(\Omega_{\mathbf{q}})} Y_{l'm'}(\Omega_{\mathbf{q}}) = \delta_{ll'} \delta_{mm'}, \quad (2.33)$$

the unitarity (2.31) becomes

$$T_l(k) - \overline{T_l(k)} = i \frac{k}{8\pi E_k} \overline{T_l(k)} T_l(k). \quad (2.34)$$

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A solution to this unitarity condition is easily obtained as

$$T_l(k) = \frac{16\pi E_k}{k} e^{i\delta_l(k)} \sin \delta_l(k), \quad (2.35)$$

where $\delta_l(k)$ is an arbitrary real function of k , and can be interpreted as the scattering phase shift, as seen later.

We now introduce the Bethe-Salpeter (BS) wave function for $\pi\pi$ system, defined by

$$\varphi(\mathbf{r}) = \langle 0 | T \{ \pi_a(\mathbf{x} + \mathbf{r}, t_a) \pi_b(\mathbf{x}, t_b) \} | k_a, a, k_b, b; \text{in} \rangle \quad (2.36)$$

where $|k_a, a, k_b, b; \text{in}\rangle$ is a $\pi\pi$ asymptotic in-state in the center of mass system such that $k_a = (E_k, \mathbf{k})$ and $k_b = (E_k, -\mathbf{k})$ with flavors a and b . The pion interpolating operator is given by

$$\pi_a(\mathbf{x}, x_0) = \bar{q}(x) i\gamma_5 \tau_a q(x), \quad q(x) = \begin{pmatrix} u(x) \\ d(x) \end{pmatrix} \quad (2.37)$$

with the Pauli matrix τ_a . For simplicity we take $t_a = t_b + \epsilon$ with $\epsilon \geq 0$ and the $\epsilon \rightarrow 0$ limit. We then simply write

$$\varphi(\mathbf{r}) = \langle 0 | \pi_a(\mathbf{x} + \mathbf{r}, t) \pi_b(\mathbf{x}, t) | k_a, a, k_b, b; \text{in} \rangle. \quad (2.38)$$

The name, the Bethe-Salpeter wave function, comes from the fact that this quantity satisfies the Bethe-Salpeter equation (Bethe and Salpeter, 1951). Unlike field equations such as the Dyson-Schwinger equations, the BS equation is derived from the diagrammatic consideration. We here consider the BS wave function from the different point of view.

By inserting the complete set of the out-states such that

$$\mathbf{1} = \sum_c \int \frac{d^3\mathbf{p}}{(2\pi)^3 2p_0} | \mathbf{p}, c; \text{out} \rangle \langle \mathbf{p}, c; \text{out} | + \sum_X \frac{| X; \text{out} \rangle \langle X; \text{out} |}{2E_X}, \quad (2.39)$$

we have

$$\varphi(\mathbf{r}) = \varphi^{\text{elastic}}(\mathbf{r}) + \varphi^{\text{inelastic}}(\mathbf{r}) \quad (2.40)$$

where

$$\varphi^{\text{elastic}}(\mathbf{r}) = \sqrt{Z_\pi} \int \frac{d^3\mathbf{p}}{(2\pi)^3 2p_0} e^{i\mathbf{p} \cdot (\mathbf{x} + \mathbf{r}) - ip_0 t} \langle \mathbf{p}, a; \text{out} | \pi_b(\mathbf{x}, t) | \mathbf{k}, a, -\mathbf{k}, b; \text{in} \rangle \quad (2.41)$$

$$\varphi^{\text{inelastic}}(\mathbf{r}) = \sum_X \langle 0 | \pi_a(\mathbf{x} + \mathbf{r}, t) | X; \text{out} \rangle \frac{1}{2E_X} \langle X; \text{out} | \pi_b(\mathbf{x}, t) | \mathbf{k}, a, -\mathbf{k}, b; \text{in} \rangle \quad (2.42)$$

and $| \mathbf{p}, a, ; \text{out} \rangle$ is an one-pion out-state with momentum \mathbf{p} , which satisfies

$$\langle 0 | \pi_a(\mathbf{x}, x_0) | \mathbf{p}, b; \text{out} \rangle = \delta_{ab} \sqrt{Z_\pi} e^{-ip \cdot x}, \quad p_0 = \sqrt{\mathbf{p}^2 + m_\pi^2}. \quad (2.43)$$

On the other hand, X represents general states other than one-pion states.

Using the reduction formula that

$$a_{\text{out}}(\mathbf{p})T(O) - T(O)a_{\text{in}}(\mathbf{p}) = (-p^2 + m_\pi^2)T(\pi(p)O) \quad (2.44)$$

$$T(O)a_{\text{in}}^\dagger(\mathbf{p}) - a_{\text{out}}^\dagger(\mathbf{p})T(O) = (-p^2 + m_\pi^2)T(O\pi^\dagger(p)) \quad (2.45)$$

where O is an arbitrary field operator and

$$\pi(p) = \int d^4x \frac{e^{ipx}}{\sqrt{Z_\pi}} \pi(x), \quad (2.46)$$

we obtain

$$\begin{aligned} \langle \mathbf{p}, a; \text{out} | \pi_b(\mathbf{x}, t) | \mathbf{k}, a, -\mathbf{k}, b; \text{in} \rangle &= \sqrt{Z_\pi} (2\pi)^3 2k_0 \delta^{(3)}(\mathbf{p} - \mathbf{k}) e^{-ikx} \\ &+ \sqrt{Z_\pi} \frac{e^{-iqx}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}(p, q, k_a, k_b) \end{aligned} \quad (2.47)$$

where off-shell T-matrix \hat{T} is defined by

$$\hat{T}(p, q, k_a, k_b) = (-p^2 + m_\pi^2)(-q^2 + m_\pi^2)G(p, q, k_a, k_b)(-k_a^2 + m_\pi^2)(-k_b^2 + m_\pi^2) \quad (2.48)$$

$$G(p, q, k_a, k_b) i(2\pi)^4 \delta^{(4)}(p + q - k_a - k_b) = \langle 0 | T \{ \pi_a(p) \pi_b(q) \pi_a^\dagger(k_a) \pi_b^\dagger(k_b) \} | 0 \rangle. \quad (2.49)$$

Here $p = (\mathbf{p}, p_0)$, $k_a = (\mathbf{k}, k_0)$ and $k_b = (-\mathbf{k}, k_0)$ are on-shell 4-momenta, while $q = (-\mathbf{p}, 2k_0 - p_0)$ is generally off-shell. Using this expression we obtain

$$\varphi^{\text{elastic}}(\mathbf{r}) = Z_\pi e^{-i2k_0 t} e^{i\mathbf{k} \cdot \mathbf{r}} + Z_\pi e^{-i2k_0 t} \int \frac{d^3\mathbf{p}}{(2\pi)^3 2p_0} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}(p, q, k_a, k_b) \quad (2.50)$$

Similarly we have

$$\varphi^{\text{inelastic}}(\mathbf{r}) = e^{-i2k_0 t} \sum_X \frac{\sqrt{Z_\pi Z_X}}{2E_X} \frac{e^{i\mathbf{p}_X \cdot \mathbf{r}}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}_X(p_X, q, k_a, k_b) \quad (2.51)$$

where $q = (-\mathbf{p}_X, 2k_0 - (p_X)_0)$. For simplicity we hereafter set $t = 0$. We rescale φ^{elastic} as

$$\varphi(\mathbf{r}) = Z_\pi \varphi^{\text{elastic}}(\mathbf{r}) + \varphi^{\text{inelastic}}(\mathbf{r}) \quad (2.52)$$

where

$$\varphi^{\text{elastic}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{p^2 - k^2 - i\varepsilon} H(\mathbf{p}, \mathbf{k}) e^{i\mathbf{p} \cdot \mathbf{r}} \quad (2.53)$$

with

$$H(\mathbf{p}, \mathbf{k}) = \frac{p_0 + k_0}{8p_0 k_0} T(\mathbf{p}, \mathbf{q}), \quad (2.54)$$

and $k = |\mathbf{k}|$ and $p = |\mathbf{p}|$.

10 Phase Shift from Lattice QCD: Lüscher's formula in the finite volume

We now investigate the large $r = |\mathbf{r}|$ behavior of the BS wave function below the 4π inelastic threshold. We first consider φ^{elastic} . Using the following partial wave decomposition

$$H(\mathbf{p}, \mathbf{k}) = 4\pi \sum_{l,m} H_l(p, k) Y_{lm}(\Omega_{\mathbf{p}}) \overline{Y_{lm}(\Omega_{\mathbf{k}})} \quad (2.55)$$

$$\varphi^{\text{elastic}}(\mathbf{r}) = 4\pi \sum_{l,m} i^l \varphi_l^{\text{elastic}}(r, k) Y_{lm}(\Omega_{\mathbf{r}}) \overline{Y_{lm}(\Omega_{\mathbf{k}})} \quad (2.56)$$

$$e^{i\mathbf{p}\cdot\mathbf{r}} = 4\pi \sum_{l,m} i^l j_l(pr) Y_{lm}(\Omega_{\mathbf{r}}) \overline{Y_{lm}(\Omega_{\mathbf{p}})}, \quad (2.57)$$

we have

$$\varphi_l^{\text{elastic}}(r, k) = j_l(kr) + \int \frac{p^2 dp}{2\pi^2} \frac{1}{p^2 - k^2 - i\varepsilon} H_l(p, k) j_l(pr). \quad (2.58)$$

We assume that the interaction vanishes for large r :

$$-(\nabla^2 + k^2)\varphi^{\text{elastic}}(\mathbf{r}) = \int \frac{d^3p}{(2\pi)^3} H(\mathbf{p}, \mathbf{k}) e^{i\mathbf{p}\cdot\mathbf{r}} \xrightarrow{r \rightarrow \infty} 0, \quad (2.59)$$

which, in terms of the partial wave, gives

$$\int \frac{p^2 dp}{2\pi^2} H_l(p, k) j_l(pr) \xrightarrow{r \rightarrow \infty} 0. \quad (2.60)$$

We evaluate the second term of eq.(2.58). Using the explicit form of the spherical Bessel function $j_l(x)$ in eq.(2.21) we have

$$\begin{aligned} \int \frac{p^2 dp}{2\pi^2} \frac{1}{p^2 - k^2 - i\varepsilon} H_l(p, k) j_l(pr) &= (-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \int_0^\infty \frac{p^{2-l} dp}{4\pi^2 i p r} \frac{e^{ipr} - e^{-ipr}}{p^2 - k^2 - i\varepsilon} H_l(p, k) \\ &= (-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \int_{-\infty}^\infty \frac{p^{2-l} dp}{4\pi^2 i p r} \frac{e^{ipr}}{p^2 - k^2 - i\varepsilon} H_l(p, k) \end{aligned} \quad (2.61)$$

Here we used the property that $H_l(-p, k) = (-1)^l H_l(p, k)$, which is shown as

$$\begin{aligned} H(\mathbf{p}, \mathbf{k}) &= 4\pi \sum_{l,m} H_l(p, k) Y_{lm}(\Omega_{\mathbf{p}}) \overline{Y_{lm}(\Omega_{\mathbf{k}})} = 4\pi \sum_{l,m} H_l(-p, k) Y_{lm}(\Omega_{-\mathbf{p}}) \overline{Y_{lm}(\Omega_{\mathbf{k}})} \\ &= 4\pi \sum_{l,m} (-1)^l H_l(-p, k) Y_{lm}(\Omega_{\mathbf{p}}) \overline{Y_{lm}(\Omega_{\mathbf{k}})} \end{aligned} \quad (2.62)$$

where $\Omega_{-\mathbf{p}}$ means $\theta \rightarrow \pi - \theta$ and $\phi \rightarrow \pi + \phi$. To proceed, we assume $H_l(p, k) = O(p^l)$ for small p , so that no contribution around $p = 0$ appears in the above integral.

We know that the half off-shell T-matrix $H_l(p, k)$ do not have any poles and cuts in the real axis, since k^2 is smaller than inelastic threshold. For simplicity we assume that

$H_l(p, k)$ has only poles in the complex p plain (this argument may also be generalized for cuts):

$$H_l(p, k) = \sum_{n>0, \text{Im}k_n>0} \frac{Z_n}{p - k_n} + \sum_{n<0, \text{Im}k_n<0} \frac{Z_n}{p - k_n} + \tilde{H}_l(p, k) \quad (2.63)$$

where $\tilde{H}_l(p, k)$ is analytic in p . Note that k_n and Z_n implicitly depend on k . This form of the assumption satisfies the condition eq.(2.60), which becomes

$$(-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \sum_{n>0, \text{Im}k_n>0} \frac{k_n^{2-l} Z_n}{2\pi k_n r} e^{i(\text{Re}k_n)r} e^{-(\text{Im}k_n)r} \simeq 0, \quad (2.64)$$

for $\bar{k}_0 r \gg 1$, where $\bar{k}_0 = \min_{n>0} \text{Im} k_n > 0$. Using the assumption (2.63), we can evaluate eq.(2.61) as

$$\begin{aligned} &= \frac{4}{4\pi} H_l(k, k) (-kr)^l \left(\frac{1}{kr} \frac{d}{dkr} \right)^l \frac{e^{ikr}}{kr} + (-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \sum_{n>0} \frac{k_n^{2-l} Z_n e^{ik_n r}}{2\pi k_n r (k_n^2 - k^2)} \\ &= \frac{k}{4\pi} H_l(k, k) \{n_l(kr) + i j_l(kr)\} + (-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \sum_{n>0} \frac{k_n^{2-l} Z_n}{2\pi k_n r (k_n^2 - k^2)} e^{i(\text{Re}k_n)r} e^{-(\text{Im}k_n)r}. \end{aligned} \quad (2.65)$$

Since $\text{Im}k_n > 0$, the sum over $n > 0$ vanishes exponentially for large r which satisfies $\bar{k}_0 r \gg 1$. Similarly we can show that $\varphi^{\text{inelastic}}(\mathbf{r})$ vanishes exponentially for large r as long as k^2 is smaller than inelastic threshold.

Therefore, for large r ($\bar{k}_0 r \gg 1$), we finally obtain

$$\begin{aligned} \varphi_l(r, k) &\simeq Z_\pi \left[j_l(kr) + \frac{k}{4\pi} H_l(k, k) \{n_l(kr) + i j_l(kr)\} \right] \\ &\simeq Z_\pi \frac{e^{i\delta_l(k)}}{kr} \sin(kr + \delta_l(k) - l\pi/2) \end{aligned} \quad (2.66)$$

where the following form of the on-shell T-matrix determined from unitarity in eq.(2.35)

$$H(k, k) = \frac{4\pi}{k} e^{i\delta_l(k)} \sin \delta_l(k), \quad (2.67)$$

and the asymptotic behaviour of $j_l(x)$ and $n_l(x)$ that

$$j_l(x) \simeq \frac{\sin(x - l\pi/2)}{x}, \quad n_l(x) \simeq \frac{\cos(x - l\pi/2)}{x} \quad (2.68)$$

are used.

Note that the derivation for the large r behavior of the BS wave function in this section is similar but a little different from that in (Lin *et al.*, 2002; Aoki *et al.*, 2005b) for $\pi\pi$ and in (Ishizuka, 2009; Aoki *et al.*, 2010b) for NN , though the final results are same.

2.2 Lüscher's formula for the phase shift in the finite volume

We now consider the finite volume (Lüscher, 1991). We assume that no interaction (except exponentially small contributions) exists at $r \geq R$, where R is sufficiently large. Therefore, if the box size L is larger than $2R$, there exist a region that $R < r < L/2$ where

$$(\nabla^2 + k^2)\varphi_L(\mathbf{r}; k) = 0 \quad (2.69)$$

is satisfied for the BS wave-function $\varphi_L(\mathbf{r}; k)$, which is given by

$$\varphi_L(\mathbf{r}; k) = \langle 0 | \pi_a(\mathbf{x} + \mathbf{r}, 0) \pi_b(\mathbf{y}, 0) | k_a, a, k_b, b \rangle_L, \quad (2.70)$$

where the subscript L indicates that the state is constructed in the finite box. This wave function is expanded in terms of the BS wave function in the infinite volume, introduced in the previous sections as

$$\varphi_L(\mathbf{r}; k) = 4\pi \sum_{l,m} C_{lm}(k) \varphi_l(r, k) Y_{lm}(\Omega_{\mathbf{r}}) \quad (2.71)$$

where the coefficient $C_{lm}(k)$ is introduced to satisfy the periodic boundary condition such that $\varphi_L(\mathbf{r} + \mathbf{n}L; k) = \varphi_L(\mathbf{r}; k)$ for $\mathbf{n} = (n_x, n_y, n_z) \in \mathbf{Z}^3$. Note that

$$\varphi_l(r, k) = n_l(kr) e^{i\delta_l(k)} \sin \delta_l(k) + j_l(kr) e^{i\delta_l(k)} \cos \delta_l(k) \quad (2.72)$$

for $r \geq R$.

On the other hand, we can construct the solution of the Helmholtz equation

$$(\nabla^2 + k^2)\varphi_L(\mathbf{r}; k) = 0 \quad (2.73)$$

for $\mathbf{r} \neq 0$ with the periodic boundary condition as

$$\phi_L(\mathbf{r}; k) = \sum_{l,m} v_{lm}(k) G_{lm}(\mathbf{r}, k) \quad (2.74)$$

where

$$G_{lm}(\mathbf{r}, k) = \sqrt{4\pi} \mathbf{Y}_{lm}(\nabla) G(\mathbf{r}, k) \quad (2.75)$$

$$G(\mathbf{r}, k) = \frac{1}{L^3} \sum_{\mathbf{p} \in \Gamma} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - k^2}, \quad \Gamma = \left\{ \mathbf{p} | \mathbf{p} = \mathbf{n} \frac{2\pi}{L}, \mathbf{n} \in \mathbf{Z}^3 \right\}, \quad (2.76)$$

$$\mathbf{Y}_{lm}(\mathbf{p}) \equiv p^l Y_{lm}(\Omega_{\mathbf{p}}), \quad p = |\mathbf{p}|. \quad (2.77)$$

It is easy to see the above $\varphi_L(\mathbf{r}; k)$ satisfies both Helmholtz equation and periodic boundary condition for arbitrary $v_{lm}(k)$'s as

$$(\nabla^2 + k^2)\varphi_L(\mathbf{r}; k) = \sum_{l,m} v_{lm}(k) \sqrt{4\pi} \mathbf{Y}_{lm}(\nabla) (\nabla^2 + k^2) G(\mathbf{r}, k)$$

$$= \sum_{l,m} v_{lm}(k) \sqrt{4\pi} \mathbf{Y}_{lm}(\nabla) \delta^{(3)}(\mathbf{r}) = 0 \quad (2.78)$$

for $\mathbf{r} \neq 0$ and

$$\begin{aligned} \varphi_L(\mathbf{r} + \mathbf{n}L; k) &= \sum_{l,m} v_{lm}(k) \sqrt{4\pi} \mathbf{Y}_{lm}(\nabla) G(\mathbf{r} + \mathbf{n}L, k) \\ &= \sum_{l,m} v_{lm}(k) \sqrt{4\pi} \mathbf{Y}_{lm}(\nabla) G(\mathbf{r}, k) = \varphi_L(\mathbf{r}; k) \end{aligned} \quad (2.79)$$

The coefficient v_{lm} can be determined by comparing eq.(2.74) with eq.(2.71). We first rewrite

$$G(\mathbf{r}, k) = \frac{k}{4\pi} n_0(kr) + \sum_{l,m} \sqrt{4\pi} Y_{lm}(\Omega_{\mathbf{r}}) g_{lm}(k) j_l(kr) \quad (2.80)$$

where

$$g_{lm}(k) = \sqrt{4\pi} \frac{1}{L^3} \sum_{\mathbf{p} \in \Gamma} \frac{(ip/k)^l}{\mathbf{p}^2 - k^2} \overline{Y_{lm}(\Omega_{\mathbf{p}})}. \quad (2.81)$$

This can be easily seen as follows. Since

$$(\nabla^2 + k^2) \frac{k}{4\pi} n_0(kr) = \delta(\mathbf{r}), \quad (2.82)$$

$$G(\mathbf{r}, k) - \frac{k}{4\pi} n_0(kr) \quad (2.83)$$

satisfies the Helmholtz equation for all \mathbf{r} and is smooth at $r \rightarrow 0$, so that it can be expanded by j_l as

$$G(\mathbf{r}, k) - \frac{k}{4\pi} n_0(kr) = \sum_{l,m} \sqrt{4\pi} g_{lm}(k) j_l(kr) Y_{lm}(\Omega_{\mathbf{r}}). \quad (2.84)$$

Using

$$e^{i\mathbf{p} \cdot \mathbf{r}} = 4\pi \sum_{lm} i^l j_l(pr) Y_{lm}(\Omega_{\mathbf{r}}) \overline{Y_{lm}(\Omega_{\mathbf{p}})} \quad (2.85)$$

in eq.(2.76), and considering the $r \rightarrow 0$ limit in the both side of eq. (2.84), we obtain eq.(2.81). (Note that $j_l(x) \simeq x^l/(2l+1)!!$ as $x \rightarrow 0$.)

We next observe(Lüscher, 1991) that

$$G_{lm}(\mathbf{r}, k) = \sqrt{4\pi} \mathbf{Y}_{lm}(\nabla) G(\mathbf{r}, k) = \frac{(-k)^l k}{4\pi}$$

Table 2.1 Non-zero independent elements of $\mathbf{M}_{lm,l'm'}$.

$\mathbf{M}_{lm,l'm'}$	$a (M_{00})$	$b (M_{40})$	$c (M_{60})$
$\mathbf{M}_{00,00}$	1	0	0
$\mathbf{M}_{1m,1m}$	1	0	0
$\mathbf{M}_{20,20}$	1	18/7	0
$\mathbf{M}_{21,21}$	1	-12/7	0
$\mathbf{M}_{22,22}$	1	3/7	0
$\mathbf{M}_{22,2-2}$	0	15/7	0
$\mathbf{M}_{30,10}$	0	$-4\sqrt{21}/7$	0
$\mathbf{M}_{31,11}$	0	$3\sqrt{14}/7$	0
$\mathbf{M}_{33,1-1}$	0	$\sqrt{210}/7$	0
$\mathbf{M}_{30,30}$	1	18/11	100/33
$\mathbf{M}_{31,31}$	1	3/11	-25/11
$\mathbf{M}_{32,32}$	1	-21/11	10/11
$\mathbf{M}_{32,3-2}$	0	15/11	-70/11
$\mathbf{M}_{33,33}$	1	9/11	-5/33
$\mathbf{M}_{33,3-1}$	0	$3\sqrt{15}/11$	$35\sqrt{15}/33$

$$\times \left[Y_{lm}(\Omega_{\mathbf{r}}) n_l(kr) + \sum_{l',m'} \mathbf{M}_{lm,l'm'} Y_{l'm'}(\Omega_{\mathbf{r}}) j_{l'}(kr) \right], \quad (2.86)$$

where non-zero elements of $\mathbf{M}_{lm,l'm'}$ are given by the linear combination of

$$M_{lm} = \frac{1}{i^l(2l+1)} \frac{4\pi}{k} g_{lm}(k). \quad (2.87)$$

The following properties generally hold:

$$\mathbf{M}_{lm,l'm'} = \mathbf{M}_{l'm',lm} = \mathbf{M}_{l-m,l'-m'}. \quad (2.88)$$

Non-zero elements at $l, l' \leq 3$ are expressed as

$$\mathbf{M}_{lm,l'm'} = aM_{00} + bM_{40} + cM_{60}, \quad (2.89)$$

with a, b, c given in table 2.1. See Ref.(Lüscher, 1991) for more details.

We now consider the cubic group $O(3, \mathbf{Z})$, which has 24 elements and is generated by following elements in the special cubic group $SO(3, \mathbf{Z})$

$$R_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad R_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad R_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (2.90)$$

and the parity transformation $P\mathbf{r} = -\mathbf{r}$. There are five irreducible representations in $SO(3, \mathbf{Z})$, denoted by A_1 , A_2 , E , T_1 and T_2 , whose dimensions are 1,1,2,3, and 3, respectively. The irreducible representations of $O(3, \mathbf{Z})$ are constructed these five

Table 2.2 Decomposition of the angular momentum into irreducible representations of the cubic group

l	rep.	basis polynomials	independent elements
0	A_1^+	1	
1	T_1^-	r_i	$i = 1, 2, 3$
2	E^+	$r_i^2 - r_j^2$	$(i, j) = (1, 2), (2, 3)$
2	T_2^+	$r_i r_j$	$i \neq j$
3	A_2^-	$r_1 r_2 r_3$	
3	T_1^-	$5r_i^3 - 3r^2 r_j$	$i = 1, 2, 3$
3	T_2^-	$r_i(r_j^2 - r_k^2)$	$(i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2)$
4	A_1^+	$5(r_1^4 + r_2^4 + r_3^4) - 3r^4$	
4	E^+	$7(r_i^4 - r_j^4) - 6r^2(r_i^2 - r_j^2)$	$(i, j) = (1, 2), (2, 3)$
4	T_1^+	$r_i r_j^3 - r_j r_i^3$	$i \neq j$
4	T_2^+	$7(r_i r_j^3 + r_j r_i^3) - 6r^2 r_i r_j$	$i \neq j$

irreducible representations of $SO(3, \mathbf{Z})$ and the parity eigenvalue ± 1 . It is noted that irreducible representations of the rotational group $O(3, \mathbf{R})$ are decomposed in terms of these irreducible representations. For example,

$$\begin{aligned} \mathbf{0} &= A_1^+, \quad \mathbf{1} = T_1^-, \quad \mathbf{2} = E^+ \oplus T_2^+, \\ \mathbf{3} &= A_2^- \oplus T_1^- \oplus T_2^-, \quad \mathbf{4} = A_1^+ \oplus E^+ \oplus T_1^+ \oplus T_2^+, \end{aligned} \quad (2.91)$$

where a number denotes an eigenvalue of the angular momentum l . The corresponding basis polynomials for each cubic representation are given in table 2.2.

We now compare two expressions of $\varphi_L(\mathbf{r}; k)$ in some irreducible representations of the cubic group. If we project the BS wave function to A_1^+ representation, which contains the $l = 0$ partial wave as well as $l \geq 4$ contribution. Neglecting $l \geq 4$ contribution, eq.(2.71) becomes

$$\varphi_L^{A_1^+}(\mathbf{r}; k) = \sqrt{4\pi} C_{00}(k) e^{i\delta_0(k)} [n_0(kr) \sin \delta_0(k) + j_0(kr) \cos \delta_0(k)] \quad (2.92)$$

for $r \geq R$. In order to match this expression, eq.(2.74) must be

$$\begin{aligned} \varphi_L^{A_1^+}(\mathbf{r}; k) &= \sqrt{4\pi} v_{00}(k) G_{00}(\mathbf{r}, k) \\ &= \sqrt{4\pi} v_{00} \left[n_0(kr) + \sum_{lm} \mathbf{M}_{00,lm} Y_{lm}(\Omega_{\mathbf{r}}) j_l(kr) \right], \end{aligned} \quad (2.93)$$

since $G_{lm}(\mathbf{r}, k)$ with $l \neq 0$, which contains $n_l(kr)$, can not appear in this equation. By comparing the two, we have

$$C_{00}(k) e^{i\delta_0(k)} \sin \delta_0(k) = v_{00} \quad (2.94)$$

$$C_{00}(k) e^{i\delta_0(k)} \cos \delta_0(k) = v_{00} \mathbf{M}_{00,00} = v_{00} M_{00}, \quad (2.95)$$

which leads to the famous Lüscher's formula (Lüscher, 1991),

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$$\cot(\delta_0(k)) = M_{00} = \frac{4\pi}{k} g_{00}(k) = \frac{4\pi}{k} \frac{1}{L^3} \sum_{\mathbf{p} \in \Gamma} \frac{1}{\mathbf{p}^2 - k^2}. \quad (2.96)$$

Note that un-matched components proportional to $\mathbf{M}_{00,4m}$ ($m = 0, \pm 4$) give $l = 4$ contributions.

Let us briefly explain how to use this formula. We first calculate the energy $E_2(L)$ of two pions in the center of mass frame on the finite L^3 box with the periodic boundary condition, where L is assumed to be larger than $2R$. We then determine k , the magnitude of the relative momentum of the two pions, from the equation that

$$E_2(L) = 2\sqrt{k^2 + m_\pi^2}, \quad (2.97)$$

where m_π is the pion mass in the infinite volume limit. We finally determine $\delta_0(k)$, by solving eq.(2.96) with k from eq.(2.97) and the spatial size L . It should be noted that the momentum for one pion is quantized as $\mathbf{p} = 2\pi\mathbf{n}/L$ on the finite box with the periodic boundary condition. If an interaction between two pions were absent, we would have $E_2(L) = 2\sqrt{\mathbf{p}^2 + m_\pi^2}$, so that $k = |\mathbf{p}|$. The presence of the interaction makes k a little different from $|\mathbf{p}|$ on the finite box. The above Lüscher's formula relates the difference to the scattering phase shift. By applying the formula for two pions with different \mathbf{p} and L , we can determine the scattering phase shift $\delta_0(k)$ at several values of k .

Similarly as above, we consider the T_1^- representation, which contains the $l = 1$ partial wave as well as $l \geq 3$ contributions. If latter ones are neglected, we again obtain

$$\cot(\delta_1(k)) = M_{00} = \frac{4\pi}{k} g_{00}(k). \quad (2.98)$$

On the other hand, if the contribution from $l = 3$ partial wave can not be neglected, in addition to the $l = 1$ component, we have

$$\begin{aligned} \varphi_L^{T_1^-}(\mathbf{r}; k) &= 4\pi \sum_m C_{1m}(k) Y_{1m}(\Omega_{\mathbf{r}\mathbf{r}}) e^{i\delta_1(k)} [n_1(kr) \sin \delta_1(k) + j_1(kr) \cos \delta_1(k)] \\ &\quad + 4\pi \sum_m C_{3m}(k) Y_{3m}(\Omega_{\mathbf{r}}) e^{i\delta_3(k)} [n_3(kr) \sin \delta_3(k) + j_3(kr) \cos \delta_3(k)], \end{aligned} \quad (2.99)$$

which should be compared with

$$\varphi_L^{T_1^-}(\mathbf{r}; k) = \sum v_{1m}(k) G_{1m}(\mathbf{r}, k) + \sum v_{3m}(k) G_{3m}(\mathbf{r}, k). \quad (2.100)$$

From the matching condition we obtain, after a little algebra,

$$\det \begin{pmatrix} \mathbf{M}_{10,10} - \cot \delta_1(k), & \mathbf{M}_{30,10} \\ \mathbf{M}_{30,10}, & \mathbf{M}_{30,30} - \cot \delta_3(k) \end{pmatrix} = 0, \quad (2.101)$$

for $m = 0$, and

$$\det \begin{pmatrix} \mathbf{M}_{11,11} - \cot \delta_1(k), & \mathbf{M}_{31,11}, & \mathbf{M}_{33,1-1} \\ \mathbf{M}_{31,11}, & \mathbf{M}_{31,31} - \cot \delta_3(k), & \mathbf{M}_{33,3-1} \\ \mathbf{M}_{33,1-1}, & \mathbf{M}_{33,3-1}, & \mathbf{M}_{33,33} - \cot \delta_3(k) \end{pmatrix} = 0, \quad (2.102)$$

for $m = 1, -3$ or $m = -1, 3$, while we have

$$\det \begin{pmatrix} \mathbf{M}_{32,32} - \cot \delta_3(k), & \mathbf{M}_{32,3-2} \\ \mathbf{M}_{32,3-2}, & \mathbf{M}_{32,32} - \cot \delta_3(k) \end{pmatrix} = 0, \quad (2.103)$$

for $m = 2, -2$. From the last equation, we can determine $\delta_3(k)$ at some k and L . Putting this $\delta_3(k)$ into the first or the second equation, we can also extract $\delta_1(k)$.

2.3 Some references for the $\pi\pi$ phase shift from lattice QCD

The BS wave function for the $\pi\pi$ system in the isospin $I = 2$ channel has been investigated in quenched QCD at $k \simeq 0$ (Aoki *et al.*, 2005a) to extract the scattering length a_0 through the Lüscher's formula in the center of mass system. The scattering length is related to the scattering phase shift $\delta_0(k)$ as

$$\frac{k}{\tan \delta_0(k)} = \frac{1}{a_0} + r_0 \frac{k^2}{2} + \mathcal{O}(k^4), \quad (2.104)$$

where r_0 is called the effective range. The calculation of the BS wave function for the $\pi\pi$ system in the $I = 2$ channel has been extended to the case of the non-zero momentum in quenched QCD (Sasaki and Ishizuka, 2008) and the $I = 2$ $\pi\pi$ scattering phase shift can be extracted using the Lüscher's formula in the laboratory system (Rummukainen and Steven Gottlieb, 1995).

Besides quenched calculations, there are only a few calculations for the $\pi\pi$ scattering phase shift.

The $I = 2$ $\pi\pi$ scattering length and phase shift have been calculated through the Lüscher's formula in 2-flavor lattice QCD with the $\mathcal{O}(a)$ improved Wilson fermion in both center of mass and laboratory systems (Yamazaki *et al.*, 2004). Both chiral and continuum extrapolations have been taken, though the pion masses in the simulation are rather heavy.

The $I = 2$ $\pi\pi$ scattering length has been calculated in the 2+1-flavor mixed action lattice QCD, using the domain-wall valence quarks with the asqtad-improved staggered sea quarks for $m_\pi^{\text{see}} \simeq 294, 348$ and 484 MeV at $a \simeq 0.125$ fm (Beane *et al.*, 2006; Beane *et al.*, 2008). The scattering phase shift has also been calculated at $k \simeq 544$ MeV and $m_\pi \simeq 484$ MeV.

Recently the $I = 2$ $\pi\pi$ scattering length has been calculated in 2-flavor twisted mass lattice QCD for pion masses ranging from 270 MeV to 485 MeV at $a \simeq 0.086$ fm (Feng *et al.*, 2010). The lattice spacing error is estimated at $a \simeq 0.067$ fm for one pion mass.

The P -wave scattering phase shift for the $I = 1$ $\pi\pi$ system has been calculated in 2-flavor lattice QCD with an improved Wilson fermion at $a = 0.22$ fm in the laboratory system (Aoki *et al.*, 2007). Since $m_\pi/m_\rho \simeq 0.41$ in this calculation, the decay width of ρ meson can be estimated from the scattering phase shift.

3

Nuclear Potential from Lattice QCD

In the previous section, we have explained the Lüscher's method to extract the scattering phase shift from the two particle energy in the finite box, considering the $\pi\pi$ case as an example. To show the relation between the phase shift and the two particle energy in the finite box, we use the fact that the BS wave function in the large separation such that $r \geq R$, where R is the interaction range between two particles in the infinite volume, satisfies the free Schrödinger equation (the Helmholtz equation) with the periodic boundary condition.

In this section, instead of the large distance behaviour, we consider the short distance properties of the BS wave function, from which we define the "potential" between two particles. We mainly consider the NN potential, though the method in this section can be applied to any two particles in principle.

3.1 Strategy to extract potentials in quantum field theories

In this subsection, we describe the strategy to extract the NN potentials in QCD (Ishii *et al.*, 2007; Aoki *et al.*, 2008; Aoki *et al.*, 2010b).

As a preparation, we introduce the T -matrix of the NN scattering below the $NN\pi$ inelastic threshold. The 4×4 T -matrix component for a given total angular momentum J is decomposed into two 1×1 submatrices and one 2×2 submatrix as (Ishizuka, 2009; Aoki *et al.*, 2010b)

$$T^J = \begin{pmatrix} T_{l=J,s=0}^J & 0 & 0_{1 \times 2} \\ 0 & T_{l=J,s=1}^J & 0_{1 \times 2} \\ 0_{2 \times 1} & 0_{2 \times 1} & T_{l=J \mp 1,s=1}^J \end{pmatrix} \quad (3.1)$$

where l is the orbital angular momentum between two nucleons and s is the total spin. The unitarity tells us that

$$T_{l=J,s}^J = \hat{T}_{Js}, \quad T_{l=J \mp 1,s=1}^J = O(k) \begin{pmatrix} \hat{T}_{J-1,1}^{-1} & 0 \\ 0 & \hat{T}_{J+1,1} \end{pmatrix} O^{-1}(k) \quad (3.2)$$

with

$$\hat{T}_{ls} = \frac{16\pi E_K}{k} e^{i\delta_{ls}(k)} \sin \delta_{ls}(k), \quad O(k) = \begin{pmatrix} \cos \epsilon_J(k) & -\sin \epsilon_J(k) \\ \sin \epsilon_J(k) & \cos \epsilon_J(k) \end{pmatrix}, \quad (3.3)$$

where $\delta_{ls}(k)$ is the scattering phase shift, whereas $\epsilon_J(k)$ is the mixing angle between $l = J \pm 1$. Here the total energy of the two nucleons is given by $2E_k = 2\sqrt{k^2 + m_N^2}$ in the center of mass frame.

Let us start describing the strategy to extract the potential in QCD. We first define the BS amplitude for two nucleons in the center of mass frame as

$$\varphi_{\alpha\beta}^E(\mathbf{r}) = \langle 0 | T \{ N_\alpha(\mathbf{y}, 0) N_\beta(\mathbf{x}, 0) \} | \mathbf{k}, s_a, -\mathbf{k}, s_b; \text{in} \rangle, \quad (3.4)$$

where the relative coordinate denoted as $\mathbf{r} = \mathbf{x} - \mathbf{y}$, the special momentum and the helicity for incoming nucleon is denoted by (\mathbf{k}, s_a) or $(-\mathbf{k}, s_b)$, the total energy $E = 2E_k$ with $k = |\mathbf{k}|$. The local composite nucleon operator is given by

$$\begin{aligned} N_\alpha^f(x) &= \epsilon^{abc} q_\alpha^{a,f}(x) q_\beta^{b,g}(x) (i\tau_2)_{gh} (C\gamma_5)^{\beta\gamma} q_\gamma^{c,h}(x) \\ &= \epsilon^{abc} q_\alpha^{a,f}(x) [q^b(x) i\tau_2 C\gamma_5 q^c(x)], \end{aligned} \quad (3.5)$$

where $q_\alpha^{a,f}$ is a quark field with the color index a , the flavor index f and the spinor index α . Here repeated index assumes a sum, $C = \gamma_2\gamma_4$ is the charge conjugation matrix and $i\tau_2$ acts on the flavor index. Unless necessary, the flavor indices are implicit.

Let us briefly consider the meaning of the BS wave function. By writing

$$\langle 0 | T \{ N(\mathbf{y}, 0) N(\mathbf{x}, 0) \} = \sum_{n,m=0}^{\infty} \int \frac{dE}{2E} \langle 2N, n(\bar{N}N), m\pi, E | f_{nm}(\mathbf{r}, E) \quad (3.6)$$

where $|2N, n(\bar{N}N), m\pi, E\rangle$ is an in-state containing two nucleons, n pairs of nucleon-antinucleon and m pions with the total energy E , we see that $\varphi^E(\mathbf{r}) = f_{00}(\mathbf{r}, E)$. (Our normalization is $\langle 2N, n(\bar{N}N), m\pi, E | | 2N, n'(\bar{N}N), m'\pi, E' \rangle = 2E\delta(E-E')\delta_{nn'}\delta_{mm'}$.) Therefore the BS wave function $\varphi^E(\mathbf{r})$ is an amplitude to find the in-state $|2N, E\rangle$ in $T \{ N(\mathbf{y}, 0) N(\mathbf{x}, 0) \} | 0 \rangle$.

As in the case of $\pi\pi$, the asymptotic behaviours of the BS wave function at $r = |\mathbf{r}| > R$, where R is the interaction range of two nucleons, agree with those of the scattering wave of the quantum mechanics (Ishizuka, 2009; Aoki *et al.*, 2010b). The BS wave function for a given total angular momentum J has 4 components. For example, the BS wave function for $l = J, s = 0$ at large r becomes

$$\begin{aligned} \varphi_{l=J,s=0}(\mathbf{r}; k) &\xrightarrow{r>R} ZY_{JJ_z}(\Omega_{\mathbf{r}}) e^{i\delta_{J0}(k)} (j_J(kr) \cos \delta_{J0}(k) + n_J(kr) \sin \delta_{J0}(k)) \\ &\simeq ZY_{JJ_z}(\Omega_{\mathbf{r}}) \frac{e^{i\delta_{J0}(k)}}{kr} \sin(kr + \delta_{J0}(k) - \pi J/2). \end{aligned} \quad (3.7)$$

where J_z is the z component of the total angular momentum. See Refs. (Ishizuka, 2009; Aoki *et al.*, 2010b) for more details. This shows that the BS wave function can be regarded as the NN scattering wave.

Now we define the non-local NN "potential" through $\varphi^E(\mathbf{r})$ (Ishii *et al.*, 2007; Aoki *et al.*, 2008; Aoki *et al.*, 2010b) as

$$\left(\frac{k^2}{2\mu} - H_0 \right) \varphi_{\alpha\beta}^E(\mathbf{x}) = \int d^3y U_{\alpha\beta,\gamma\delta}(\mathbf{x}, \mathbf{y}) \varphi_{\gamma\delta}^E(\mathbf{y}), \quad H_0 = \frac{-\nabla^2}{2\mu}, \quad (3.8)$$

where $\mu = m_N/2$ is the reduced mass of the two nucleons. It is noted that $U(\mathbf{x}, \mathbf{y})$ is non-local but energy-independent and this potential is equivalent to the local but energy dependent potential $V(\mathbf{r}, \mathbf{k})$, which is defined by

$$K(\mathbf{r}, \mathbf{k}) \equiv \left(\frac{k^2}{2\mu} - H_0 \right) \varphi(\mathbf{r}, \mathbf{k}) = V(\mathbf{r}, \mathbf{k}) \varphi(\mathbf{x}, \mathbf{k}), \quad (3.9)$$

where we write $\varphi(\mathbf{r}, \mathbf{k}) = \varphi^E(\mathbf{r})$. To see the equivalence, we construct the dual basis $\tilde{\varphi}(\mathbf{k}, \mathbf{r})$ as

$$\tilde{\varphi}(\mathbf{k}, \mathbf{r}) = \int d^3p \, \eta^{-1}(\mathbf{k}, \mathbf{p}) \overline{\varphi(\mathbf{r}, \mathbf{p})}, \quad (3.10)$$

where the metric is given by

$$\eta(\mathbf{k}, \mathbf{p}) = \int d^3r \, \overline{\varphi(\mathbf{r}, \mathbf{k})} \varphi(\mathbf{r}, \mathbf{p}). \quad (3.11)$$

It is easy to see that the dual basis satisfies

$$\int d^3y \, \tilde{\varphi}(\mathbf{k}, \mathbf{r}) \varphi(\mathbf{r}, \mathbf{p}) = \delta^{(3)}(\mathbf{k} - \mathbf{p}) \quad (3.12)$$

$$\int d^3p \, \varphi(\mathbf{x}, \mathbf{p}) \tilde{\varphi}(\mathbf{p}, \mathbf{y}) = \delta^{(3)}(\mathbf{x} - \mathbf{y}). \quad (3.13)$$

Using the dual basis, we obtain the non-local potential from the local one as

$$U(\mathbf{x}, \mathbf{y}) = \int d^3p \, K(\mathbf{x}, \mathbf{p}) \tilde{\varphi}(\mathbf{p}, \mathbf{y}) = \int d^3p \, V(\mathbf{x}, \mathbf{p}) \varphi(\mathbf{x}, \mathbf{p}) \tilde{\varphi}(\mathbf{p}, \mathbf{y}). \quad (3.14)$$

This establishes one to one correspondence between the non-local but energy-independent potential $U(\mathbf{x}, \mathbf{y})$ and the local but energy-dependent one $V(\mathbf{r}, \mathbf{k})$.

The equivalence also tells us that we need to know the BS wave function at all energies to completely construct $U(\mathbf{x}, \mathbf{y})$. Although this is principle possible, it is in practice very difficult. We therefore consider the following derivative expansion of $U(\mathbf{x}, \mathbf{y})$.

$$U(\mathbf{x}, \mathbf{y}) = V(\mathbf{x}, \nabla) \delta^{(3)}(\mathbf{x} - \mathbf{y}). \quad (3.15)$$

The structure of the $V(\mathbf{r}, \nabla)$ can be determined as follows (Okubo and Marshak, 1958). The most general (non-relativistic) NN potential is parameterized as

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}_1, \mathbf{p}_2, \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2, t) \quad (3.16)$$

where \mathbf{r}_i , \mathbf{p}_i , $\vec{\sigma}_i$ and $\vec{\tau}_i$ are the coordinate, the momentum, the spin and the isospin of the i -th nucleon, respectively and the t is the time. There are several conditions this potential should satisfy.

1. Probability conservation implies the hermiticity of the potential, $V^\dagger = V$.
2. Eneregy conservation imply the t independence while the momentum conservation says that the potential depends on the combination $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ only.
3. Galilei invariance tells us that the potential contains $\mathbf{p} = \mathbf{p}_1 - \mathbf{p}_2$ only. From these three conditions, we have $V = V(\mathbf{r}, \mathbf{p}, \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2)$.

4. The total angular momentum conservation implies that V is invariant under $\vec{J} = \vec{L} + \vec{S}$ with the orbital angular momentum $\vec{L} = \mathbf{r} \times \mathbf{p}$ and the total spin $\vec{S} = (\vec{\sigma}_1 + \vec{\sigma}_2)/2$.
5. The potential should be invariant under parity, $(\mathbf{r}, \mathbf{p}, \vec{\sigma}_i) \rightarrow (-\mathbf{r}, -\mathbf{p}, \vec{\sigma}_i)$.
6. The potential is invariant under time-reversal, $(\mathbf{r}, \mathbf{p}, \vec{\sigma}_i) \rightarrow (\mathbf{r}, -\mathbf{p}, -\vec{\sigma}_i)$.
7. Quantum statistics of the exchange of two nucleons implies the invariance of the potential under $(\mathbf{r}, \mathbf{p}, \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2) \rightarrow (-\mathbf{r}, -\mathbf{p}, \vec{\sigma}_2, \vec{\sigma}_1, \vec{\tau}_2, \vec{\tau}_1)$.
8. From isospin invariance, V contains only $\mathbf{1} \cdot \mathbf{1}$ or $\vec{\tau}_1 \cdot \vec{\tau}_2$ in the isospin space.
9. The potential has only $\vec{\sigma}_1^n \vec{\sigma}_2^m$ terms with $(n, m) = (0, 0), (1, 0), (0, 1), (1, 1)$. The other higher order terms can be reduced to these terms because of the property that $\sigma^i \sigma^j = \delta^{ij} + i\epsilon^{ijk} \sigma^k$.

The terms which contain Pauli matrices and satisfy the above conditions are constructed as

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2, (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{L}, (\vec{\sigma}_1 \cdot \mathbf{r})(\vec{\sigma}_2 \cdot \mathbf{r}), (\vec{\sigma}_1 \cdot \mathbf{p})(\vec{\sigma}_2 \cdot \mathbf{p}), (\vec{\sigma}_1 \cdot \vec{L})(\vec{\sigma}_2 \cdot \vec{L}), \quad (3.17)$$

which are customarily reorganized as

$$\begin{aligned} \vec{\sigma}_1 \cdot \vec{\sigma}_2, \quad S_{12} &\equiv 3(\vec{\sigma}_1 \cdot \hat{\mathbf{r}})(\vec{\sigma}_2 \cdot \hat{\mathbf{r}}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2, \quad \vec{L} \cdot \vec{S}, \\ P_{12} &\equiv (\vec{\sigma}_1 \cdot \mathbf{p})(\vec{\sigma}_2 \cdot \mathbf{p}), \quad W_{12} \equiv Q_{12} - \frac{1}{3} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{L}^2, \end{aligned} \quad (3.18)$$

where S_{12} is called the tensor operator, and

$$Q_{12} \equiv \frac{1}{2} \left[(\vec{\sigma}_1 \cdot \vec{L})(\vec{\sigma}_2 \cdot \vec{L}) + (\vec{\sigma}_2 \cdot \vec{L})(\vec{\sigma}_1 \cdot \vec{L}) \right], \quad (3.19)$$

Finally we obtain

$$V = \sum_{I=1,2} V^I(\mathbf{r}, \mathbf{p}, \vec{\sigma}_1, \vec{\sigma}_2) P_I^T \quad (3.20)$$

where

$$V^I = V_0^I + V_\sigma^I(\vec{\sigma}_1 \cdot \vec{\sigma}_2) + V_{LS}^I(\vec{L} \cdot \vec{S}) + \frac{1}{2} \{V_T^I, S_{12}\} + \frac{1}{2} \{V_P^I, P_{12}\} + \frac{1}{2} \{V_W^I, W_{12}\} \quad (3.21)$$

with coefficient functions $V_X^I = V_X^I(\mathbf{r}^2, \mathbf{p}^2, \vec{L}^2)$ for $I = 0, 1$ and $X = 0, \sigma, T, LS, P, W$. Here P_I^T is the projection operator to the state with the total isospin I , given by

$$P_{I=0}^T = \frac{1}{4} - \vec{\tau}_1 \cdot \vec{\tau}_2, \quad P_{I=1}^T = \frac{3}{4} + \vec{\tau}_1 \cdot \vec{\tau}_2. \quad (3.22)$$

The anticommutators in Eq.(3.21) are necessary to make the potential hermitian, since S_{12} , P_{12} and W_{12} do not commute with the scalar potentials $V_X^I(\mathbf{r}^2, \mathbf{p}^2, \vec{L}^2)$.

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From the general consideration above, we have, for example at $O(\nabla)$,

$$V(\mathbf{r}, \nabla) = \sum_{I=0,1} \left[V_0^I(r) + V_\sigma^I(r) \vec{\sigma}_1 \cdot \vec{\sigma}_2 + V_T^I(r) S_{12} + V_{LS}^I(r) \vec{L} \cdot \vec{S} \right] P_I^T + O(\nabla^2). \quad (3.23)$$

This form of the potential has often been used in nuclear physics. Note that the first 3 terms are $O(1)$ while the LS potential is $O(\nabla)$.

This is the strategy to define and extract the NN potential in QCD. There are two important and mutually-related remarks.

The leading order potential in the derivative expansion is nothing but the local potential $V(\mathbf{r}, \mathbf{k})$. By construction, this (local) potential reproduces the correct phase shift $\delta(k)$ at $k = |\mathbf{k}|$, while it is not guaranteed that this potential gives the correct phase shift at different $k' = |\mathbf{k}'| (\neq k)$. This means that the local potential $V(\mathbf{r}, \mathbf{k})$ and $V(\mathbf{r}, \mathbf{k}')$ may differ, and this energy dependence of the local potential gives a measure for the non-locality of the non-local but energy independent potential $U(\mathbf{x}, \mathbf{y})$ because of the equivalence between V and U . If the the first order in the derivative expansion is good at low energy, we expect that energy dependence of the potential V is expected to be small at small k .

Secondly it should be mentioned that the potential U defined through the BS amplitude of course depends on the choice of the interpolating field operators $N(x)$. In principle, one may choose any (local) composite operators with the same quantum numbers as the nucleon to define the BS wave function. Different choices for the nucleon operator give different BS wave functions, which may leads to different NN potentials, though they all gives the same scattering phase shift. While the potential is not an physical observable in this sense, it does not mean that it is useless, however. The strategy in this report gives one specific scheme for the NN potential in QCD, which is defined through the BS amplitude constructed from the local nucleon field without derivatives. This is quite analogous to the situation for the running coupling in QCD. Although the running coupling is scheme-dependent, it is useful to understand and describe the deep inelastic proton-electron scattering. Let us make this analogy more concrete. A physical observables is the scattering data in both cases, the deep inelastic scattering or the NN scattering. An example of the physical interpretation is the almost free partons in proton for the case of the deep inelastic scattering, while it is an existence of the repulsive core for the case of NN scattering. An theoretical explanation for the phenomena is the asymptotic freedom of the QCD running coupling for the free partons, while no valid theoretical explanation exists so far for the repulsive core. In this report, we introduce one definite scheme for the potential based on QCD, in order to show an existence of the repulsive core. Although the choice of the scheme is irrelevant in principle, it is better to use a "good" scheme in practice. In the case of the running coupling, good convergence of the perturbative expansion may give one criterion, though the popularly used $\overline{\text{MS}}$ coupling may not be the best one for this criterion. In the case of the NN potential, on the other hand, good convergence of the derivative expansion may give a criteria for a "good" potential. In other words, the good potential is almost local and energy-independent. The NN potential which

is completely local and energy-independent at all energy range is therefore the best one. It is also unique if the inverse scattering method holds for the NN case.

3.2 Extraction of the BS wave function on the lattice

In this subsection, we explain how to extract the BS wave function from correlation functions on the lattice. For simplicity, we here consider the $l = 0$ state, namely the S -state.

The BS wave function on the lattice with the lattice spacing a and the spatial lattice volume L^3 is extracted from the 4-point correlation function, by inserting the complete set of the QCD eigenstates in the finite box as,

$$G_{\alpha\beta}(\mathbf{x}, \mathbf{y}, t - t_0; J^P) = \langle 0 | n_\beta(\mathbf{y}, t) p_\alpha(\mathbf{x}, t) \bar{J}_{pn}(t_0; J^P) | 0 \rangle \quad (3.24)$$

$$= \sum_{n=0}^{\infty} A_n \langle 0 | n_\beta(\mathbf{y}, t) p_\alpha(\mathbf{x}, t) | E_n \rangle e^{-E_n(t-t_0)} \quad (3.25)$$

$$\xrightarrow{t \gg t_0} A_0 \varphi_{\alpha\beta}(\mathbf{r}; J^P), \quad \mathbf{r} = \mathbf{x} - \mathbf{y} \quad (3.26)$$

with the matrix element $A_n = \langle E_n | \bar{J}_{pn}(0) | 0 \rangle$, where p (n) is the proton (neutron) interpolating operator, $p = N^u$ ($n = N^d$), $|E_n\rangle$ is the QCD eigenstate with the baryon number 2 and the total energy $E_n = 2\sqrt{k_n^2 + m_N^2}$. The state created by the source \bar{J}_{pn} have the conserved quantum numbers, (J, J_z) (total angular momentum and its z -component), I (total isospin) and P (parity). To study the NN potential in the $J^P = 0^+$ with $I = 1$ (1S_0) channel and the $J^P = 1^+$ with $I = 0$ (3S_1 and 3D_1) channel, a wall-source located at $t = t_0$ with the Coulomb gauge fixing only at $t = t_0$ is used,

$$J_{pn}(t_0, J^P) = P_{\beta\alpha}^s [p_\alpha^{\text{wall}}(t_0) n_\beta^{\text{wall}}(t_0)] \quad (3.27)$$

where $p^{\text{wall}}(t_0)$ and $n^{\text{wall}}(t_0)$ are obtained by replacing the local quark fields $q(x)$ in $N(x)$ by the wall quark fields,

$$q^{\text{wall}}(t_0) = \sum_{\mathbf{x}} q(\mathbf{x}, t_0). \quad (3.28)$$

By construction, the source operator eq.(3.27) has zero orbital angular momentum at $t = t_0$, so that states with fixed (J, J_z) are obtained by the spin projection with $(s, s_z) = (J, J_z)$, e.g. $P_{\beta\alpha}^{s=0} = (\sigma^2)_{\beta\alpha}$ and $P_{\beta\alpha}^{s=1, s_z=0} = (\sigma^1)_{\beta\alpha}$. Note that the l and s are not separately conserved, so that the state created by the source $J_{pn}(t_0; 1^+)$ becomes a mixture of the $l = 0$ (S -state) and $l = 2$ (D -state) at later time $t > t_0$.

The BS wave function in the orbital S state is then defined with the projection operator for the cubic group P^R with the irreducible representation R and that for the spin P^s as

$$\varphi(r; ^1S_0) = P^{A_1^+} P^{s=0} \varphi(\mathbf{r}; 0^+) \equiv \frac{1}{24} \sum_{g \in O(3, \mathbf{Z})} P_{\alpha\beta}^{s=0} \varphi_{\alpha\beta}(g^{-1}\mathbf{r}; 0^+) \quad (3.29)$$

$$\varphi(r; {}^3S_1) = P^{A_1^+} P^{s=0} \varphi(\mathbf{r}; 1^+) \equiv \frac{1}{24} \sum_{g \in O(3, \mathbf{Z})} P_{\alpha\beta}^{s=1} \varphi_{\alpha\beta}(g^{-1}\mathbf{r}; 1^+), \quad (3.30)$$

where the summation over $g \in O(3, \mathbf{Z})$ is taken for the cubic transformation group with 24 elements to project out the $l = 0$ component in the A_1^+ representation, and contributions from the higher orbital waves with $l \geq 4$ contained in the A_1^+ rep. are expected to be negligible at low energy.

Form these BS wave functions, we can construct the local potentials at the leading order of the derivative expansion. For the 1S_0 channel, the central potential becomes

$$V_C(r; {}^1S_0) \equiv V_0^{I=1}(r) + V_\sigma^{I=1}(r) = \frac{k^2}{m_N} + \frac{1}{m_N} \frac{\nabla^2 \varphi(r; {}^1S_0)}{\varphi(r; {}^1S_0)} \quad (3.31)$$

while for the 3S_1 channel there are two independent terms, $V_C(r; {}^3S_1) = V_0^{I=0}(r) - 3V_\sigma^{I=0}(r)$ and $V_T^{I=0}(r)$, at the leading order. For a while we ignore V_T and define the effective central potential as

$$V_C^{\text{eff}}(r; {}^3S_1) = \frac{k^2}{m_N} + \frac{1}{m_N} \frac{\nabla^2 \varphi(r; {}^3S_1)}{\varphi(r; {}^3S_1)}, \quad (3.32)$$

where the "effective" central potential means that it includes the effect of the tensor potential V_T as the second order perturbation.

It is noted here that k^2 is determined from the total energy E_0 of two nucleons as $E_0 = 2\sqrt{k^2 + m_N^2}$.

3.3 Tensor potential

While the central potential acts separately on the S and D components, the tensor potential provides a coupling between these two components. We therefore consider a coupled-channel Schrödinger equation in the $J^P = 1^+$ channel, in which the BS wave function has both S-wave and D-wave components as

$$(H_0 + V_C(r; 1^+) + V_T(r)S_{12}) \varphi(\mathbf{r}; 1^+) = \frac{k^2}{m_N} \varphi(\mathbf{r}; 1^+). \quad (3.33)$$

The projections to the S-wave and D-wave components similar to eq. (3.30) are defined by

$$P\varphi_{\alpha\beta}(r) \equiv P^{A_1^+} \varphi_{\alpha\beta}(\mathbf{r}; 1^+), \quad (3.34)$$

$$Q\varphi_{\alpha\beta}(r) \equiv (1 - P^{A_1^+}) \varphi_{\alpha\beta}(\mathbf{r}; 1^+). \quad (3.35)$$

Here both $P\varphi_{\alpha\beta}$ and $Q\varphi_{\alpha\beta}$ contain additional components with $l \geq 4$ but they are expected to be small at low energy.

Multiplying P and Q to eq.(3.33) from the left and using the properties that H_0 , $V_C(r; 1^+)$ and $V_T(r)$ commute with P and Q , we obtain

$$H_0[P\varphi](r) + V_C(r; 1^+)[P\varphi](r) + V_T(r)[PS_{12}\varphi](r) = \frac{k^2}{m_N}[P\varphi](r) \quad (3.36)$$

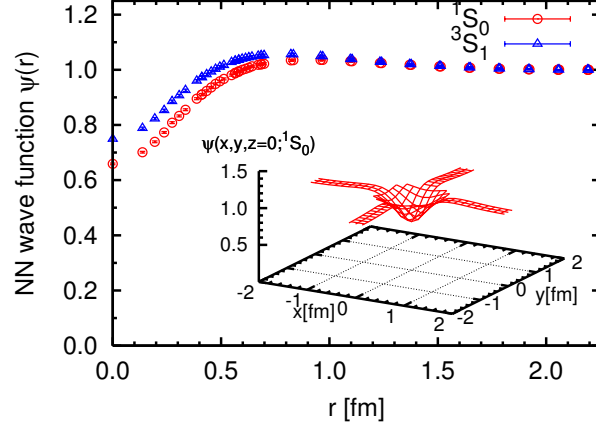


Fig. 3.1 The NN wave function in 1S_0 and 3S_1 channels at $m_\pi = 529$ MeV, measured at $(t - t_0) = 6a$. The inset is a three-dimensional plot of the wave function $\varphi(x, y, z = 0; ^1S_0)$.

$$H_0[Q\varphi](r) + V_C(r; 1^+)[Q\varphi](r) + V_T(r)[QS_{12}\varphi](r) = \frac{k^2}{m_N}[Q\varphi](r) \quad (3.37)$$

where, for simplicity, the spinor indices, α and β are suppressed. Note that S_{12} does not commute with P or Q .

By solving these equations for $(\alpha, \beta) = (2, 1)$ component, we finally extract

$$V_C(r; 1^+) = \frac{k^2}{m_N} - \frac{1}{D(r)} \{[QS_{12}\varphi]_{21}(r)H_0[P\varphi]_{21}(r) - [PS_{12}\varphi]_{21}(r)H_0[Q\varphi]_{21}(r)\} \quad (3.38)$$

$$V_T(r) = \frac{1}{D(r)} \{[Q\varphi]_{21}(r)H_0[P\varphi]_{21}(r) - [P\varphi]_{21}(r)H_0[Q\varphi]_{21}(r)\} \quad (3.39)$$

where

$$D(r) \equiv [P\varphi]_{21}(r)H_0[QS_{12}\varphi]_{21}(r) - [Q\varphi]_{21}(r)H_0[PS_{12}\varphi]_{21}(r). \quad (3.40)$$

Note that the effective central potential is expressed as

$$V_C^{\text{eff}}(r; ^3S_1) = \frac{k^2}{m_N} - \frac{H_0[P\varphi]_{21}(r)}{[P\varphi]_{21}(r)} \quad (3.41)$$

with $H_0 = -\nabla^2/m_N$.

3.4 Results in lattice QCD

The first result for the NN potential in lattice QCD based on the strategy in the previous subsections appeared in Ref.(Ishii *et al.*, 2007), where the (effective) central potential has been calculated for 1S_0 (3S_1) channel in quenched QCD simulations at

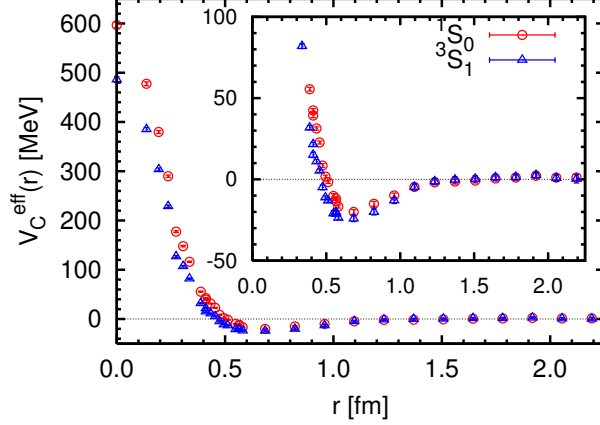


Fig. 3.2 The central potential in the 1S_0 channel and the effective central potential in the 3S_1 channels at $m_\pi = 529$ MeV.

the lattice spacing $a \simeq 0.137$ fm and the spacial extension $L \simeq 4.4$ fm. More details of numerical simulations can be found in Ref. (Ishii *et al.*, 2007).

Fig.3.1 shows the BS wave function in 1S_0 and 3S_1 channels at $m_\pi = 529$ MeV and $k^2 \simeq 0$, which is measured at $t - t_0 = 6a$. The wave functions are normalized to be 1 at the largest spatial point $r = 2.192$ fm.

The reconstructed central and effective central potentials in the 1S_0 and 3S_1 channels at $m_\pi = 529$ MeV from the BS wave functions with the formulae (3.31) and (3.32) are shown in Fig.3.2. The overall structure of the potentials are similar to the known phenomenological NN potentials discussed in Sec.1, namely the repulsive core at short distance surrounded by the attractive well at medium and long distances. The figure also shows that the interaction between two nucleons is well switched off for $r > 1.5$ fm, so that the condition $R < L/2 \simeq 2.2$ is satisfied.

To check the stability of these potentials against the time-slice adopted to define the BS wave function, the t -dependence of the 1S_0 potential for several different values of r is shown in Fig.3.3 at $m_\pi = 529$ MeV. In this case, the choice $t - t_0 = 6a$ for the extraction of $V_C(r)$ is large enough to assure the stability within statistical errors, which indicates the ground state dominance at this t .

The NN potentials in the 1S_0 channel are compared among three different quark masses in Fig.3.4. As the quark mass decreases, the repulsive core at short distance and the attractive well at medium distance becomes stronger simultaneously.

The 3S_1 and 3D_1 components of the BS wave functions obtained from $J^P = 1^+$, $J_z = 0$ state at $m_\pi = 529$ MeV and $k^2 \simeq 0$ are plotted in Fig.3.5(a), according to eqs. (3.34) and (3.35). Note that the 3D_1 wave function becomes multi-valued as a function of r due to its angular dependence. It is expected that $(\alpha, \beta) = (2, 1)$ spin component of the D-state wave function for $J^P = 1^+$ and $J_z = 0$ is proportional to the $Y_{20}(\theta, \phi) \propto 3 \cos^2 \theta - 1$. As shown in Fig.3.5(b), the D-state wave function, divided by the $Y_{20}(\theta, \phi)$, becomes almost single-valued, so that the D-wave component is indeed

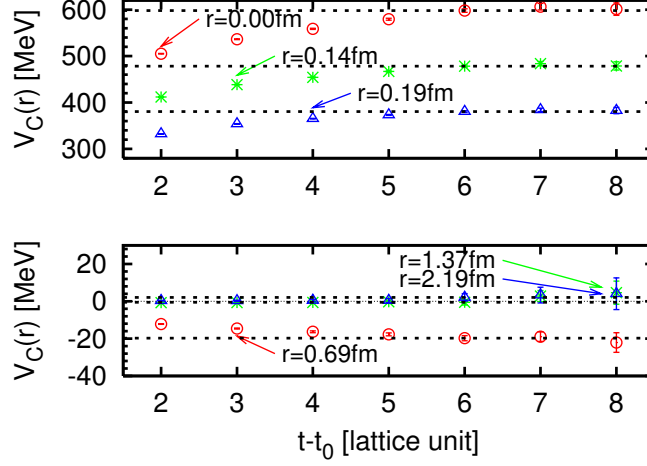


Fig. 3.3 The t dependence of the potential at $r = 0, 0.14, 0.19, 1.37, 2.19, 0.69$ fm from top to bottom in the 1S_0 channel at $m_\pi = 529$ MeV.

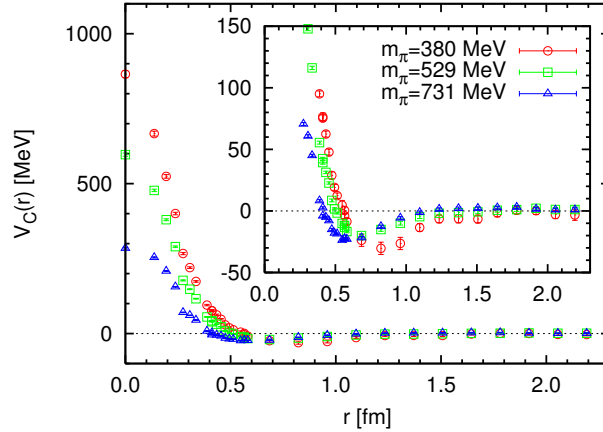


Fig. 3.4 The central potentials in the 1S_0 channel at three different quark masses.

dominant in $Q\varphi(r)$. The central potential $V_C(r; 1^+)$ and the tensor potential $V_T(r)$ together with the effective central potential $V_C^{\text{eff}}(r; ^3S_1)$ in the 3S_1 channel are plotted in Fig.3.6. Note that $V_C^{\text{eff}}(r; ^3S_1)$ contains the effect of $V_T(r)$ implicitly as higher order effects through the process such as $^3S_1 \rightarrow ^3D_1 \rightarrow ^3S_1$. In the real world, $V_C^{\text{eff}}(r; ^3S_1)$ is expected to acquire large attraction from the tensor force, which is reason why the bound state for a deuteron exist in the 3S_1 while no bound states appears for a dineutron. As seen from Fig.3.6, the difference between $V_C(r; 1^+)$ and $V_C^{\text{eff}}(r; ^3S_1)$ is still small in this quenched simulations due to relatively large quark masses.

The tensor potential $V_T(r)$ in Fig.3.6 is negative for the whole range of r within statistical errors and has a minimum at short distance around 0.4 fm. If the tensor

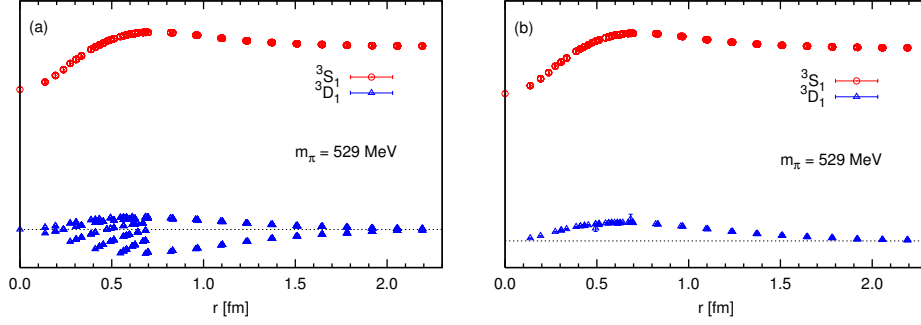


Fig. 3.5 (a) $(\alpha, \beta) = (2, 1)$ components of the S-state and the D-state wave functions projected out from a single state with $J^P = 1^+$, $J_z = 0$. (b) The D-state wave function is divided by Y_{20} .

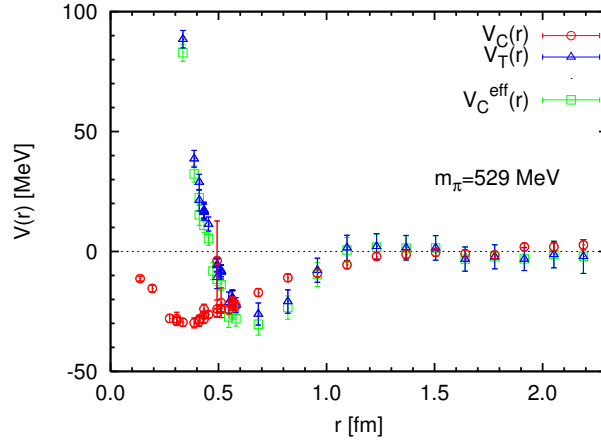


Fig. 3.6 The central potential $V_C(r; 1^+)$ and the tensor potential $V_T(r)$ obtained from the J^+ BS wave function at $m_\pi = 529$ MeV, together with $V_C^{\text{eff}}(r; {}^3S_1)$.

force receives significant contribution from the one-pion exchange as expected from the meson theory, V_T would be rather sensitive to the change of the quark mass. As shown in Fig.3.7, indeed the attraction of $V_T(r)$ substantially increases as the quark mass decreases.

At present potentials are determined at leading order of the derivative expansion, and examples presented so far are extracted from lattice data taken at $k \simeq 0$. If the higher order terms such as $V_{LS}(r)\vec{L} \cdot \vec{S}$ becomes important, the LO local potentials determined at $k > 0$ are expected to be different from the one at $k \simeq 0$. From such k dependence of the LO local potentials, some of the higher order terms can in principle be determined. A lattice QCD analysis on the k dependence has been recently carried out by changing the spatial boundary condition of the quark field from the periodic to the anti-periodic ones, which corresponds to the change from $k \simeq 0$ MeV to $k =$

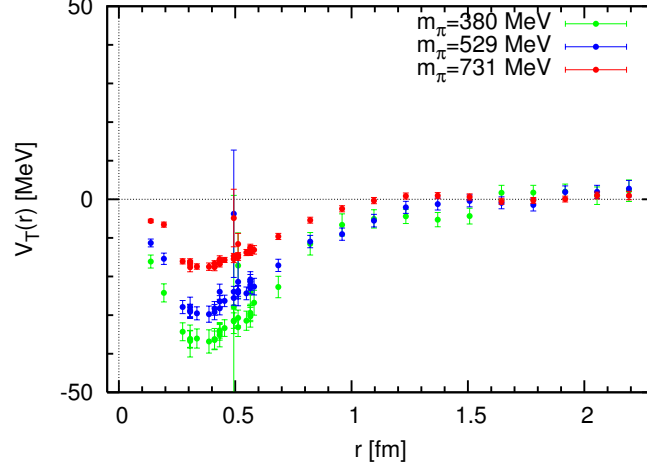


Fig. 3.7 Quark mass dependence of the tensor potential $V_T(r)$.

$\sqrt{3(\pi/L)^2} \simeq 250$ MeV. In Fig.3.8, the local potential for the 1S_0 channel obtained at $k \simeq 250$ MeV is compared with the one at $k \simeq 0$ in quenched QCD at $a = 0.137$ fm and $m_\pi = 529$ MeV. As seen from the figure, the k dependence of the local potential turns out to be very small for every r within statistical errors. Namely the non-locality of the potential with the choice of the local interpolating operator for the nucleon is small, and the present local potential at the LO can be used to well describe physical observables such as the phase shift $\delta_0(k)$ from $k \simeq 0$ to $k \simeq 250$ MeV without significant modification, at least in quenched QCD at $a = 0.137$ fm and $m_\pi = 529$ MeV. This also indicates that the definition for the potential through the BS wave function with the local nucleon operator is a "good scheme".

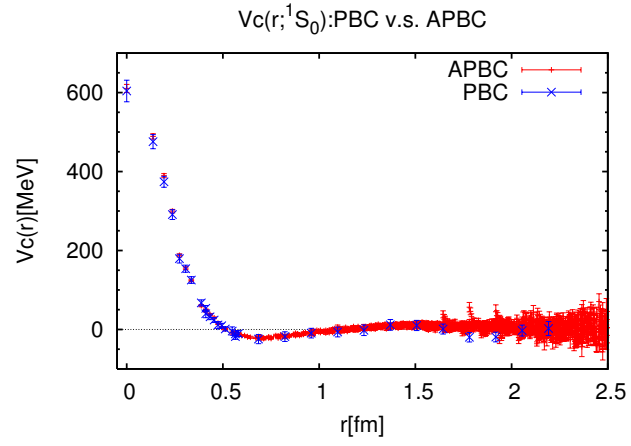


Fig. 3.8 A comparison of central potentials at $k \simeq 0$ (PBC, blue) and at $k \simeq 250$ MeV (APBC, red) for the 1S_0 state in quenched QCD at $a = 0.137$ fm and $m_\pi = 529$ MeV.

4

Repulsive core and operator product expansion in QCD

As shown in the previous section, the lattice QCD calculations shows that the NN potential defined through the BS wave function has not only the attraction at medium to long distance, which has long well been understood in terms of pion and other heavier meson exchanges, but also a characteristic repulsive core at short distance, whose origin is still theoretically unclear. A recent attempt(Aoki *et al.*, 2010a) to theoretically understand the short distance behavior of the potential in terms of the operator product expansion(OPE) is explained in this section.

4.1 Basic idea

Let us first explain the basic idea. We consider the equal time BS wave function defined by

$$\varphi_{AB}^E(\mathbf{r}) = \langle 0 | O_A(\mathbf{r}/2, 0) O_B(-\mathbf{r}/2, 0) | E \rangle \quad (4.1)$$

where $|E\rangle$ is some eigen-state of a certain system with the total energy E , and O_A , O_B are some operators of this system. We here suppress other quantum number of the state $|E\rangle$ for simplicity. The OPE reads

$$O_A(\mathbf{r}/2, 0) O_B(-\mathbf{r}/2, 0) \simeq \sum_C D_{AB}^C(\mathbf{r}) O_C(\mathbf{0}, 0), \quad (4.2)$$

from which we have

$$\varphi_{AB}^E(\mathbf{r}) \simeq \sum_C D_{AB}^C(\mathbf{r}) \langle 0 | O_C(\mathbf{0}, 0) | E \rangle. \quad (4.3)$$

It is noted that \mathbf{r} dependence appears solely in $D_{AB}^C(\mathbf{r})$ while the E dependence exists only in $\langle 0 | O_C(\mathbf{0}, 0) | E \rangle$. Suppose that the coefficient function of the OPE behaves in the small $r = |\mathbf{r}|$ limit as

$$D_{AB}^C(\mathbf{r}) \simeq r^{\alpha_C} (-\log r)^{\beta_C} f_C(\theta, \phi) \quad (4.4)$$

where θ, ϕ are angles in the polar coordinate of \mathbf{r} , the BS wave function becomes

$$\varphi_{AB}^E(\mathbf{r}) \simeq \sum_C r^{\alpha_C} (-\log r)^{\beta_C} f_C(\theta, \phi) D_C(E), \quad D_C(E) = \langle 0 | O_C(\mathbf{0}, 0) | E \rangle \quad (4.5)$$

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in this limit. The potential at short distances can be known from this expression. For example, in the case of the Ising field theory in 2-dimensions, the OPE for the spin field σ is given by

$$\sigma(x, 0)\sigma(0, 0) \simeq G(r)\mathbf{1} + cr^{3/4}O_1(0) + \cdots, \quad r = |x|, \quad (4.6)$$

where $O_1(x) (=:\bar{\psi}\psi(x))$ in terms of the free fermion fields) is an operator of dimension 1, which leads to

$$\varphi(r, E) \simeq r^{3/4}D(E) + O(r^{7/4}), \quad D(E) = c\langle 0|O_1(0)|E\rangle, \quad (4.7)$$

where $|E\rangle$ is a two-particle state with energy $E = 2\sqrt{k^2 + m^2}$. From this expression the potential becomes

$$V(r) = \frac{\varphi''(r, E) + k^2\varphi(r, E)}{m\varphi(r, E)} \simeq -\frac{3}{16} \frac{1}{mr^2} \quad (4.8)$$

in the $r \rightarrow 0$ limit. The OPE predicts not only the r^{-2} behavior of the potential at short distance but also its coefficient $-3/16$. Furthermore the potential at short distance does not depend on the energy of the state in this example(Aoki *et al.*, 2009b).

As will be seen later, the dominant terms at short distance have $\alpha_C = 0$. Among these terms, we assume that C has the largest contribution such that $\beta_C > \beta_{C'}$ for $\forall C' \neq C$. Since, as will be also seen later, such dominant operators with $\alpha_C = 0$ mainly couples to the zero angular momentum ($L = 0$) state, let us consider the BS wave function with $L = 0$, given by

$$\varphi_{AB}^E(\mathbf{r}) \simeq (-\log r)^{\beta_C} D_C(E) + \sum_{C' \neq C} (-\log r)^{\beta_{C'}} D_{C'}(E). \quad (4.9)$$

Using

$$\nabla^2(-\log r)^\beta = -\beta \frac{(-\log r)^{\beta-1}}{r^2} \left[1 - \frac{\beta-1}{-\log r} \right], \quad (4.10)$$

we obtain the following classification of the short distance behavior of the potential.

1. $\beta_C \neq 0$: The potential at short distance is energy independent and becomes

$$V(r) \simeq -\frac{\beta_C}{r^2(-\log r)}, \quad (4.11)$$

which is attractive for $\beta_C > 0$ and repulsive for $\beta_C < 0$.

2. $\beta_C = 0$: In this case the potential becomes

$$V(r) \simeq \frac{D_{C'}(E) - \beta_{C'}}{D_C(E)} \frac{(-\log r)^{\beta_{C'}-1}}{r^2}, \quad (4.12)$$

where $\beta_{C'} < 0$ is the second largest one. The sign of the potential at short distance depends on the sign of $D_{C'}(E)/D_C(E)$.

On the lattice, we do not expect divergence at $r = 0$ due to lattice artifacts at short distance. The above classification hold at $a \ll r \ll 1/\Lambda_{\text{QCD}}$, while the potential becomes finite even at $r = 0$ on the lattice.

4.2 Renormalization group analysis and operator product expansion

In N_f -flavor QCC regularized in $D = 4 - 2\epsilon$, bare local composite operators $O_A^{(0)}(x)$ are renormalized as

$$O_A^{(\text{ren})}(x) = Z_{AB}(g, \epsilon) O_B^{(0)}(x), \quad (4.13)$$

We here ignore the contribution from quark mass terms, which generates less singular terms in the OPE. Throughout this section, summation of repeated indices is assumed. The meaning of this formula is that finite results are obtained if we insert the right hand side into any correlation function, provided the QCD coupling and the quark and gluon fields are appropriately renormalized. We first consider an n -quark correlation function without operator insertion $G_n^{(0)}(g_0, \epsilon)$ (Here the dependence on the quark momenta and other quantum numbers suppressed.), which is renormalized as

$$G_n^{(\text{ren})}(g, \mu) = Z_F^{-n/2}(g, \epsilon) G_n^{(0)}(g_0, \epsilon), \quad (4.14)$$

where the coupling renormalization is given by

$$g_0^2 = \mu^{2\epsilon} Z_1(g^2, \epsilon) g^2. \quad (4.15)$$

The renormalization constant Z_1 in the minimal subtraction (MS) scheme has only pure poles terms as

$$Z_1(g^2, \epsilon) = 1 - \frac{\beta_0 g^2}{\epsilon} - \frac{\beta_1 g^4}{2\epsilon} + \frac{\beta_0^2 g^4}{\epsilon^2} + O(g^6) \quad (4.16)$$

where

$$\beta_0 = \frac{1}{16\pi^2} \left\{ \frac{11N}{3} - \frac{2N_f}{3} \right\}, \quad \beta_1 = \frac{1}{256\pi^4} \left\{ \frac{34N^2}{3} - \left(\frac{13N}{3} - \frac{1}{N} \right) N_f \right\}. \quad (4.17)$$

Similarly the quark field renormalization constant is given by

$$Z_F(g, \epsilon) = 1 - \frac{\gamma_{F0} g^2}{2\epsilon} + O(g^4). \quad (4.18)$$

The gluon field renormalization constant is also similar but is not necessary for our purpose. Similarly an n -quark correlation function with operator insertion $G_{n;A}^{(0)}(g_0, \epsilon)$ is renormalized as

$$G_{n;A}^{(\text{ren})}(g, \mu) = Z_{AB}(g, \epsilon) Z_F^{-n/2}(g, \epsilon) G_{n;B}^{(0)}(g_0, \epsilon), \quad (4.19)$$

where

$$Z_{AB}(g, \epsilon) = \delta_{AB} - \frac{\gamma_{AB}^{(1)} g^2}{2\epsilon} + O(g^4). \quad (4.20)$$

The renormalization group (RG) equations are obtained from the simple fact that bare quantities are independent of the renormalization scale μ . Introducing the RG differential operator

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$$D(\mu) = \mu \frac{\partial}{\partial \mu} + \beta_D(g) \frac{\partial}{\partial g} \quad (4.21)$$

the RG equation for n -quark correlation functions can be written as

$$\left\{ D(\mu) + \frac{n}{2} \gamma_F(g) \right\} G_n^{(\text{ren})}(g, \mu) = 0, \quad (4.22)$$

where the RG beta function is

$$\beta_D(g) \equiv \mu \frac{\partial g}{\partial \mu} = - \frac{\epsilon g}{1 + \frac{g}{2} \frac{\partial \ln Z_1}{\partial g}} = -\epsilon g - \beta_0 g^3 - \beta_1 g^5 + \mathcal{O}(g^7), \quad (4.23)$$

while the RG gamma function for quark fields is

$$\gamma_F(g) = \beta_D(g, \epsilon) \frac{\partial \ln Z_F}{\partial g} = \gamma_{F0} g^2 + \mathcal{O}(g^4). \quad (4.24)$$

Note that $\beta_D(g)$ differs from $\beta_4(g)$ only by $-\epsilon g$, and therefore has the smooth limit to $D = 4$. The RG invariant Λ parameter satisfies $D(\mu)\Lambda = 0$ with the Ansatz that

$$\Lambda = \mu e^{f(g)}. \quad (4.25)$$

The solution is the lambda-parameter in the MS scheme, Λ_{MS} , if the arbitrary integration constant is fixed by requiring that for small coupling

$$f(g) = -\frac{1}{2\beta_0 g^2} - \frac{\beta_1}{2\beta_0^2} \ln(\beta_0 g^2) + \mathcal{O}(g^2). \quad (4.26)$$

Finally the RG equations for n -quark correlation functions with operator insertion are of the form

$$\left\{ D(\mu) + \frac{n}{2} \gamma_F(g) \right\} G_{n;A}^{(\text{ren})}(g, \mu) - \gamma_{AB}(g) G_{n;B}^{(\text{ren})}(g, \mu) = 0, \quad (4.27)$$

where

$$\gamma_{AB}(g) = -Z_{AC} \beta_D(g, \epsilon) \frac{\partial Z_{CB}^{-1}}{\partial g} = \gamma_{AB}^{(1)} g^2 + \mathcal{O}(g^4). \quad (4.28)$$

Let us consider the OPE

$$O_1(y/2) O_2(-y/2) \simeq D_B(y) O_B(0). \quad (4.29)$$

where O_1 and O_2 are nucleon operators and the set of operators O_B are local 6-quark operators of canonical dimension 9 and higher. All operators in (4.29) are renormalized ones, but from now on we suppress the labels $^{(\text{ren})}$. As we will see, the nucleon operators are renormalized diagonally as

$$O_1 = Z_1(g, \epsilon) O_1^{(0)}, \quad O_2 = Z_2(g, \epsilon) O_2^{(0)}, \quad (4.30)$$

and the corresponding RG gamma functions are defined by

$$\gamma_{1,2}(g) = \beta_D(g, \epsilon) \frac{\partial \ln Z_{1,2}}{\partial g} = \gamma_{1,2}^{(1)} g^2 + O(g^4). \quad (4.31)$$

Comparing (4.29) with its bare version,

$$O_1^{(0)}(y/2) O_2^{(0)}(-y/2) \simeq D_B^{(0)}(y) O_B^{(0)}(0), \quad (4.32)$$

we can read off the renormalization of the coefficient functions as

$$D_B(y) = Z_1(g, \epsilon) Z_2(g, \epsilon) D_A^{(0)}(y) Z_{AB}^{-1}(g, \epsilon) \quad (4.33)$$

so the the RG equation becomes

$$D(\mu) D_B(g, \mu, y) + D_A(g, \mu, y) \tilde{\gamma}_{AB}(g) = 0, \quad (4.34)$$

where the effective gamma function matrix is defined as

$$\tilde{\gamma}_{AB}(g) = \gamma_{AB}(g) - [\gamma_1(g) + \gamma_2(g)] \delta_{AB}. \quad (4.35)$$

Hereafter we assume the dimensionless coefficient functions, which can be written as $D_A(g, \mu, y) = D_A(g; \mu r)$ with $r = |y|$. For the case of operators with higher canonical dimension $9 + \alpha$ the coefficients are of the form r^α times dimensionless functions and the analysis is completely analogous and can be done independently, since in the massless theory operators of different dimension do not mix. In the full theory quark mass terms are also present, but they correspond to higher powers in r and therefore can be neglected.

To solve the vector partial equation (4.34), we introduce $\hat{U}_{AB}(g)$, the solution of the matrix ordinary differential equation

$$\beta(g) \frac{d}{dg} \hat{U}_{AB}(g) = \tilde{\gamma}_{AC}(g) \hat{U}_{CB}(g) \quad (4.36)$$

and its matrix inverse $U_{AB}(g)$. With this solution, $D_B(g; \mu r)$ can be easily obtained as

$$D_B(g; \mu r) = F_A(\Lambda r) U_{AB}(g), \quad (4.37)$$

where the vector F_A is RG-invariant. Now the running coupling \bar{g} is introduced as the solution of the equation

$$f(\bar{g}) = f(g) + \ln(\mu r) = \ln(\Lambda r). \quad (4.38)$$

Note that \bar{g} is a function of r but does not depend on μ . Since F_B is RG invariant, we can evaluate it at $\mu = 1/r$ as

$$F_B(\Lambda r) = D_A(\bar{g}; 1) \hat{U}_{AB}(\bar{g}). \quad (4.39)$$

By definition $g = \bar{g}$ at $\mu = 1/r$. Since, because of asymptotic freedom (AF), for $r \rightarrow 0$ also $\bar{g} \rightarrow 0$ as

$$\bar{g}^2 \approx -\frac{1}{2\beta_0 \ln(\Lambda r)}, \quad (4.40)$$

F_B can be calculated perturbatively.

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Putting everything together, the operator product expansion (4.29) can be rewritten as

$$O_1(y/2)O_2(-y/2) \simeq F_B(\Lambda r) \tilde{O}_B(0), \quad (4.41)$$

where

$$\tilde{O}_B = U_{BC}(g) O_C. \quad (4.42)$$

There is a factorization of the operator product into perturbative and non-perturbative quantities: $F_B(\Lambda r)$ is perturbative and calculable (for $r \rightarrow 0$) thanks to AF, whereas the matrix elements of \tilde{O}_B are non-perturbative but r -independent.

The coefficient functions have the perturbative expression

$$D_A(g; \mu r) = D_{A;0} + g^2 D_{A;1}(\mu r) + O(g^4), \quad (4.43)$$

and the basis of operators can be chosen such that the 1-loop mixing matrix is diagonal:

$$\tilde{\gamma}_{AB}(g) = 2\beta_0 \beta_A g^2 \delta_{AB} + O(g^4). \quad (4.44)$$

In such a basis the solution of (4.36) in perturbation theory takes the form

$$\hat{U}_{AB}(g) = \{\delta_{AB} + R_{AB}(g)\} g^{-2\beta_B}, \quad (4.45)$$

where $R_{AB}(g) = O(g^2)$, with possible multiplicative $\log g^2$ factors, depending on the details of the spectrum of 1-loop eigenvalues β_A . An operator O_B first occurring at ℓ_B -loop order on the right hand side of (4.29) has coefficient $F_B(\Lambda r)$ with leading short distance behavior

$$F_B(\Lambda r) \approx D_{B,\ell_B}(1) \bar{g}^{2(\ell_B - \beta_B)} \approx D_{B,\ell_B}(1) (-2\beta_0 \ln(\Lambda r))^{\beta_B - \ell_B}. \quad (4.46)$$

In principle, an operator with very large β_B , even if it is not present in the expansion at tree level yet, might be important at short distances. This is why it is necessary to calculate the full 1-loop spectrum of β_B eigenvalues. As we will see, no such operators exist for the two nucleon case, and therefore operators with non-vanishing tree level coefficients are dominating at short distances. The corresponding coefficient functions have leading short distance behavior given by

$$F_B(\Lambda r) \approx D_{B;0} (-2\beta_0 \ln(\Lambda r))^{\beta_B}. \quad (4.47)$$

4.3 OPE and Anomalous dimensions for two nucleons

The general form of a gauge invariant local 3-quark operator is given by

$$B_\Gamma^F(x) \equiv B_{\alpha\beta\gamma}^{fgh}(x) = \varepsilon^{abc} q_\alpha^{a,f}(x) q_\beta^{b,g}(x) q_\gamma^{c,h}(x), \quad (4.48)$$

The color index runs from 1 to $N = 3$, the spinor index from 1 to 4, and the flavor index from 1 to N_f . A summation over a repeated index is assumed, unless otherwise stated. Note that $B_{\alpha\beta\gamma}^{fgh}$ is symmetric under any interchange of pairs of indices (e.g. $B_{\alpha\beta\gamma}^{fgh} = B_{\beta\alpha\gamma}^{ghf}$) because the quark fields anticommute. For simplicity we sometimes use the notation such as $F = fgh$ and $\Gamma = \alpha\beta\gamma$ as indicated in (4.48).

The nucleon operator is constructed from the above operators as

$$B_\alpha^f(x) = (P_{+4})_{\alpha\alpha'} B_{\alpha'\beta\gamma}^{fgh} (C\gamma_5)_{\beta\gamma} (i\tau_2)^{gh}, \quad (4.49)$$

where $P_{+4} = (1 + \gamma_4)/2$ is the projection to the large spinor component, $C = \gamma_2\gamma_4$ is the charge conjugation matrix, and τ_2 is the Pauli matrix in the flavor space (for $N_f = 2$) given by $(i\tau_2)^{fg} = \varepsilon^{fg}$. Both $C\gamma_5$ and $i\tau_2$ are anti-symmetric under the interchange of two indices, so that the nucleon operator has spin 1/2 and isospin 1/2. Although the explicit form of the γ matrices is unnecessary in principle, we find it convenient to use a chiral convention given by

$$\gamma_k = \begin{pmatrix} 0 & i\sigma_k \\ -i\sigma_k & 0 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}, \quad \gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}. \quad (4.50)$$

As discussed in the previous subsection, the OPE at the tree level (generically) dominates at short distance. The OPE of two nucleon operators given above at tree level becomes

$$B_\alpha^f(x + y/2) B_\beta^g(x - y/2) = B_\alpha^f(x) B_\beta^g(x) + \frac{y^\mu}{2} \left\{ \partial_\mu [B_\alpha^f(x)] B_\beta^g(x) - B_\alpha^f(x) \partial_\mu [B_\beta^g(x)] \right\} + \mathcal{O}(y^2). \quad (4.51)$$

For the two-nucleon operator with either the combination $[\alpha\beta]$, $\{fg\}$ ($S = 0$) or the combination $\{\alpha\beta\}$, $[fg]$ ($S = 1$), terms odd in y vanish in the above OPE, so that only even L contributions appear. These 6-quark operators are anti-symmetric under the exchange $(\alpha, f) \leftrightarrow (\beta, g)$. On the other hand, for two other operators with $([\alpha\beta], [fg])$ or $(\{\alpha\beta\}, \{fg\})$, which are symmetric under the exchange, terms even in y vanish in the OPE and only odd L 's contribute.

Knowing the anomalous dimensions of the 6-quark operators appearing in the OPE, which will be calculated later in this subsection, the OPE at short distance ($r = |\mathbf{y}| \ll 1$, $y_4 = 0$) becomes

$$B_\alpha^f(x + y/2) B_\beta^g(x - y/2) \simeq \sum_A c_A(r) O_{\alpha\beta}^{fg,A}(x) + \sum_B d_B(r) y^k O_{\alpha\beta,k}^{fg,B}(x) + \mathcal{O}(r^2), \quad (4.52)$$

where the coefficient functions behave as

$$c_A(r) \simeq (-\log r)^{\beta_A}, \quad d_B(r) \simeq (-\log r)^{\beta_B}, \quad (4.53)$$

and $\beta_{A,B}$ are related to the anomalous dimensions of the 6-quark operators $O_{\alpha\beta}^{fg,A}$ and of those with one derivative $O_{\alpha\beta,k}^{fg,B}$. The wave function defined through the eigenstate $|E\rangle$ is given by

$$\varphi_E^{\text{even}}(y) = \langle 0 | B_\alpha^f(x + y/2) B_\beta^g(x - y/2) | E \rangle \simeq \sum_A c_A(r) \langle 0 | O_{\alpha\beta}^{fg,A}(x) | E \rangle \quad (4.54)$$

for the anti-symmetric states, while

$$\varphi_E^{\text{odd}}(y) = \langle 0 | B_\alpha^f(x + y/2) B_\beta^g(x - y/2) | E \rangle \simeq \sum_B d_B(r) y^k \langle 0 | O_{\alpha\beta,k}^{fg,B}(x) | E \rangle \quad (4.55)$$

for the symmetric states. Hereafter we consider only 6-quark operators without derivatives and calculate the corresponding anomalous dimensions.

The renormalization factor Z_X of a k -quark operator $X = [q^k]$ is defined through the relation

$$[q^k]^{\text{ren}} = Z_X [q_0^k] = Z_X Z_F^{k/2} [q^k], \quad (4.56)$$

where $q_0(q)$ is the bare (renormalized) quark field. The wave function renormalization factor for the quark field is given at 1-loop by

$$Z_F = 1 + g^2 Z_F^{(1)}, \quad Z_F^{(1)} = -\frac{\lambda C_F}{16\pi^2 \epsilon} \quad (4.57)$$

where λ is the gauge parameter and $C_F = \frac{N^2-1}{2N}$.

At 1-loop the renormalization of simple k -quark operators without gauge fields is given by the divergent parts of diagrams involving exchange of a gluon between any pair of quark fields. The 1-loop correction to the insertion of an operator $q_\alpha^{a,f}(x) q_\beta^{b,g}(x)$ in any correlation function involving external quarks is expressed as the contraction of

$$q_\alpha^{a,f}(x) q_\beta^{b,g}(x) \frac{1}{2!} \int d^D y d^D z A_\mu^A(y) A_\nu^B(z) [\bar{q}^{f_1}(y) i g T^A \gamma_\mu q^{f_1}(y)] [\bar{q}^{g_1}(z) i g T^B \gamma_\nu q^{g_1}(z)] \quad (4.58)$$

where $\text{tr } T^A T^B = \delta^{AB}/2$ in our normalization. Since two identical contributions cancel the $2!$ in the denominator, the contraction at 1-loop is given by

$$-g^2 (T^A)_{aa_1} (T^A)_{bb_1} \int d^D y d^D z [S_F(x-y) \gamma_\mu q(y)]_{\alpha}^{a_1 f_1} G_{\mu\nu}(y-z) \times [S_F(x-z) \gamma_\nu q(z)]_{\beta}^{b_1 g_1} \quad (4.59)$$

where the free quark and gauge propagators are given in momentum space as

$$S_F(p) = \frac{-i\not{p} + m}{p^2 + m^2}, \quad G_{\mu\nu}(k) = \frac{1}{k^2} \left[g_{\mu\nu} - (1-\lambda) \frac{k_\mu k_\nu}{k^2} \right]. \quad (4.60)$$

The above contribution can be written as

$$\frac{g^2}{2N} \{ \delta_{aa_1} \delta_{bb_1} - N \delta_{ab_1} \delta_{a_1 b} \} \int \frac{d^D p d^D q}{(2\pi)^{2D}} T_{\alpha\alpha_1, \beta\beta_1}(p, q) q_{\alpha_1}^{a_1 f_1}(p) e^{ipx} q_{\beta_1}^{b_1 g_1}(q) e^{iqx} \quad (4.61)$$

where

$$T_{\alpha\alpha_1, \beta\beta_1}(p, q) = \int \frac{d^D k}{(2\pi)^D} [S_F(p+k) \gamma_\mu]_{\alpha\alpha_1} G_{\mu\nu}(k) [S_F(q-k) \gamma_\nu]_{\beta\beta_1}, \quad (4.62)$$

whose divergent part is independent of the momenta p, q and is given by

$$T_{\alpha\alpha_1, \beta\beta_1}(0, 0) = \frac{1}{16\pi^2} \frac{1}{\epsilon} \left[-\frac{1}{4} \sum_{\mu\nu} \sigma_{\mu\nu} \otimes \sigma_{\mu\nu} + \lambda \mathbf{1} \otimes \mathbf{1} \right]_{\alpha\alpha_1, \beta\beta_1} \quad (4.63)$$

with $\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]$. The divergent part of the 1-loop contribution becomes

$$\left[q_\alpha^{a,f}(x) q_\beta^{b,g}(x) \right]^{1-\text{loop, div}} = \frac{g^2}{32N\pi^2} \frac{1}{\epsilon} [(\mathbf{T}_0 + \lambda \mathbf{T}_1) \cdot q^a(x) \otimes q^b(x)]_{\alpha, \beta}^{fg} \quad (4.64)$$

where (bold-faced symbols represent matrices in flavor and spinor space)

$$(\mathbf{T}_0)_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1} = -\frac{1}{4} \sum_{\mu\nu} \{ \mathbf{s}_{\mu\nu} \otimes \mathbf{s}_{\mu\nu} + N \mathbf{s}_{\mu\nu} \tilde{\otimes} \mathbf{s}_{\mu\nu} \}_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1}, \quad (4.65)$$

$$(\mathbf{T}_1)_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1} = \{ \mathbf{1} \otimes \mathbf{1} + N \mathbf{1} \tilde{\otimes} \mathbf{1} \}_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1}. \quad (4.66)$$

Here we use the notation

$$\{ \mathbf{X} \otimes \mathbf{Y} \}_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1} = \mathbf{X}_{\alpha\alpha_1}^{ff_1} \mathbf{Y}_{\beta\beta_1}^{gg_1}, \quad \{ \mathbf{X} \tilde{\otimes} \mathbf{Y} \}_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1} = \mathbf{X}_{\beta\alpha_1}^{gf_1} \mathbf{Y}_{\alpha\beta_1}^{fg_1}, \quad (4.67)$$

$$\{ \mathbf{s}_{\mu\nu} \}_{\alpha\beta}^{fg} = \delta^{fg} (\sigma_{\mu\nu})_{\alpha\beta}, \quad \{ \mathbf{1} \}_{\alpha\beta}^{fg} = \delta^{fg} \delta_{\alpha\beta}. \quad (4.68)$$

By the following Fierz identities for spinor indices

$$-\frac{1}{4} \sum_{\mu\nu} \sigma_{\mu\nu} \otimes \sigma_{\mu\nu} = P_R \otimes P_R + P_L \otimes P_L - 2(P_R \tilde{\otimes} P_R + P_L \tilde{\otimes} P_L), \quad (4.69)$$

$$-\frac{1}{4} \sum_{\mu\nu} \sigma_{\mu\nu} \tilde{\otimes} \sigma_{\mu\nu} = P_R \tilde{\otimes} P_R + P_L \tilde{\otimes} P_L - 2(P_R \otimes P_R + P_L \otimes P_L), \quad (4.70)$$

where P_R, P_L are the chiral projectors, $P_R = (1 + \gamma_5)/2$ and $P_L = (1 - \gamma_5)/2$, \mathbf{T}_0 can be simplified as

$$(\mathbf{T}_0)_{\alpha\alpha_1, \beta\beta_1}^{ff_1, gg_1} = \delta^{ff_1} \delta^{gg_1} [\delta_{\alpha\alpha_1} \delta_{\beta\beta_1} - 2\delta_{\beta\alpha_1} \delta_{\alpha\beta_1}] + N \delta^{gf_1} \delta^{fg_1} [\delta_{\beta\alpha_1} \delta_{\alpha\beta_1} - 2\delta_{\alpha\alpha_1} \delta_{\beta\beta_1}] \quad (4.71)$$

where either $\alpha_1, \beta_1 \in \{1, 2\}$ (right-handed) or $\alpha_1, \beta_1 \in \{3, 4\}$ (left-handed) due to the chiral projections in eqs. (4.69) and (4.70). In the following calculation of the 1-loop anomalous dimensions, eq. (4.64) together with eqs. (4.71) and (4.66) are the key equations.

We now calculate the anomalous dimensions of general 3-quark operators at 1-loop. In terms of the renormalization factor defined as

$$B_3^{\text{renor.}} = Z_{3q} [q_0^3] = Z_{3q} Z_F^{3/2} [q^3], \quad Z_{3q} = 1 + g^2 (Z_{3q}^{(1)} + Z_{3q, \lambda}^{(1)}) + \dots, \quad (4.72)$$

where $Z_{3q}^{(1)}$ ($Z_{3q, \lambda}^{(1)}$) is the λ -independent (dependent) part at 1-loop, the divergent part of the insertion of the 3-quark operator $B_\Gamma^F = B_{\alpha\beta\gamma}^{fgh}$ at 1-loop is given by a linear combination of insertion of baryon operators as

$$(\Gamma^{(1)\text{div}})_\Gamma^F = -g^2 \left(Z_{3q}^{(1)} + Z_{3q,\lambda}^{(1)} + \frac{3}{2} Z_F^{(1)} \right)_{\Gamma\Gamma'}^{FF'} B_{\Gamma'}^{F'}. \quad (4.73)$$

The λ -dependent contribution from \mathbf{T}_1 in (4.66) is diagonal and given by

$$g^2 (\Gamma_\lambda^{(1)\text{div}})_\Gamma^F = 3\lambda \frac{g^2}{32\pi^2} \frac{N+1}{N\epsilon} B_\Gamma^F, \quad (4.74)$$

so that the λ -dependent part of Z_{3q} vanishes:

$$Z_{3q,\lambda}^{(1)} = -\frac{3\lambda}{32\pi^2} \frac{N+1}{N\epsilon} - \frac{3}{2} Z_F^{(1)} = \frac{\lambda}{64N\pi^2} \frac{3(N+1)(N-3)}{\epsilon} = 0 \quad (N=3). \quad (4.75)$$

Therefore Z_{3q} is λ -independent, as expected from the gauge invariance. We leave N explicit in some formulae to keep track of the origin of the various terms, but we should always set $N=3$ at the end.

The λ -independent part of $\Gamma^{(1)}$ from \mathbf{T}_0 in (4.71) leads to ($N=3$):

$$(\Gamma^{(1)\text{div}})_{\alpha\beta\gamma}^{fgh} = \frac{(N+1)}{2N} \frac{g^2}{16\pi^2\epsilon} \left[3B_{\alpha\beta\gamma}^{fgh} - 2B_{\beta\alpha\gamma}^{fgh} - 2B_{\gamma\beta\alpha}^{fgh} - 2B_{\alpha\gamma\beta}^{fgh} \right], \quad (4.76)$$

$$(\Gamma^{(1)\text{div}})_{\alpha\beta\hat{\gamma}}^{fgh} = \frac{(N+1)}{2N} \frac{g^2}{16\pi^2\epsilon} \left[B_{\alpha\beta\hat{\gamma}}^{fgh} - 2B_{\beta\alpha\hat{\gamma}}^{fgh} \right], \quad (4.77)$$

where $\alpha, \beta, \gamma \in \{1, 2\}$ (right-handed), while $\hat{\gamma} \in \{\hat{1} = 3, \hat{2} = 4\}$ (left-handed). Note that the same results hold with hatted and unhatted indices exchanged. These results can be easily diagonalized as

$$(Z_{3q}^{(1)})_{\{\alpha\alpha\beta\}}^{fgh} = (Z_{3q}^{(1)})_{\{\hat{\alpha}\hat{\alpha}\hat{\beta}\}}^{fgh} = 12 \frac{d}{\epsilon}, \quad (4.78)$$

$$(Z_{3q}^{(1)})_{[\alpha\beta]\alpha}^{f\neq gh} = (Z_{3q}^{(1)})_{[\hat{\alpha}\hat{\beta}]\hat{\alpha}}^{f\neq gh} = -12 \frac{d}{\epsilon}, \quad (4.79)$$

$$(Z_{3q}^{(1)})_{\{\alpha\beta\}\hat{\gamma}}^{fgh} = (Z_{3q}^{(1)})_{\{\hat{\alpha}\hat{\beta}\}\gamma}^{fgh} = 4 \frac{d}{\epsilon}, \quad (4.80)$$

$$(Z_{3q}^{(1)})_{[\alpha\beta]\hat{\gamma}}^{f\neq gh} = (Z_{3q}^{(1)})_{[\hat{\alpha}\hat{\beta}]\gamma}^{f\neq gh} = -12 \frac{d}{\epsilon}, \quad (4.81)$$

where d is given by

$$d \equiv \frac{1}{32N\pi^2} = \frac{1}{96\pi^2}. \quad (4.82)$$

The square bracket denotes antisymmetrization $[\alpha\beta] = \alpha\beta - \beta\alpha$, and curly bracket means $\{\alpha\beta\} = \alpha\beta + \beta\alpha$, $\{\alpha\alpha\beta\} = \alpha\alpha\beta + \alpha\beta\alpha + \beta\alpha\alpha$. The totally symmetric case corresponds to the decuplet representation (for $N_f = 3$) and contains the $N_f = 2, I = 3/2$ representation. The antisymmetric case corresponds to the octet representation (for $N_f = 3$) and contains the $N_f = 2, I = 1/2$ representation. The anomalous dimension at 1-loop, obtained from

$$\gamma = g^2 \gamma^{(1)} + \mathcal{O}(g^4) = \beta_D(g, \epsilon) \frac{\partial \ln Z_{3q}}{\partial g} = -2Z_{3q}^{(1)} g^2 \epsilon + \mathcal{O}(g^4), \quad (4.83)$$

becomes

$$\left(\gamma^{(1)} \right)_{\{\alpha\alpha\beta\}}^{fgh} = \left(\gamma^{(1)} \right)_{\{\hat{\alpha}\hat{\alpha}\hat{\beta}\}}^{fgh} = -24d, \quad (4.84)$$

$$\left(\gamma^{(1)}\right)_{[\alpha\beta]\alpha}^{f\neq gh} = \left(\gamma^{(1)}\right)_{[\hat{\alpha}\hat{\beta}]\hat{\alpha}}^{f\neq gh} = 24d, \quad (4.85)$$

$$\left(\gamma^{(1)}\right)_{\{\alpha\beta\}\hat{\gamma}}^{fgh} = \left(\gamma^{(1)}\right)_{\{\hat{\alpha}\hat{\beta}\}\gamma}^{fgh} = -8d, \quad (4.86)$$

$$\left(\gamma^{(1)}\right)_{[\alpha\beta]\hat{\gamma}}^{f\neq gh} = \left(\gamma^{(1)}\right)_{[\hat{\alpha}\hat{\beta}]\gamma}^{f\neq gh} = 24d. \quad (4.87)$$

We next consider the renormalization of arbitrary local gauge invariant 6-quark operator of (lowest) dimension 9, which can be written as a linear combination of operators

$$O_C(x) = B_{\Gamma_1, \Gamma_2}^{F_1, F_2}(x) \equiv B_{\Gamma_1}^{F_1}(x) B_{\Gamma_2}^{F_2}(x) = O_A(x) O_B(x), \quad (4.88)$$

with $A = (\Gamma_1, F_1)$ and $B = (\Gamma_2, F_2)$. Note $O_A(x)$ and/or $O_B(x)$ may not be operators with proton or nucleon quantum numbers and separately may not be diagonally renormalizable at one loop. The reason for considering the renormalization in more generality is that in principle there may be operators in this class which occur in the OPE of two nucleon operators at higher order in PT, but are relevant in the analysis because of their potentially large anomalous dimensions.

According to the structure of the divergent part at 1-loop order, the operators in eq. (4.88) mix only with operators $O_{C'} = O_{A'} O_{B'}$ which preserve the set of flavors and Dirac indices in the chiral basis i.e.

$$F_1 \cup F_2 = F'_1 \cup F'_2, \quad \Gamma_1 \cup \Gamma_2 = \Gamma'_1 \cup \Gamma'_2.$$

Note however that such operators are not all linearly independent. Relations between them follow from a general identity satisfied by the totally antisymmetric epsilon symbol which for N labels reads

$$N \varepsilon^{a_1 \dots a_N} \varepsilon^{b_1 \dots b_N} = \sum_{j,k} \varepsilon^{a_1 \dots a_{j-1} b_k a_{j+1} \dots a_N} \varepsilon^{b_1 \dots b_{k-1} a_j b_{k+1} \dots b_N}. \quad (4.89)$$

For our special case, $N = 3$, this identity implies the following identities among the 6-quark operators

$$3B_{\Gamma_1, \Gamma_2}^{F_1, F_2} + \sum_{i,j=1}^3 B_{(\Gamma_1, \Gamma_2)[i,j]}^{(F_1 F_2)} = 0, \quad (4.90)$$

where i -th index of abc and j -th index of def are interchanged in $(abc, def)[i, j]$. For example, $(\Gamma_1, \Gamma_2)[1, 1] = \alpha_2 \beta_1 \gamma_1, \alpha_1 \beta_2 \gamma_2$ or $(\Gamma_1, \Gamma_2)[2, 1] = \alpha_1 \alpha_2 \gamma_1, \beta_1 \beta_2 \gamma_2$. Note that the interchange of indices occurs simultaneously for both Γ_1, Γ_2 and F_1, F_2 in the above formula. The plus sign in (4.90) appears because the quark fields are Grassmann.

As an example of identities, let us consider the case that $\Gamma_1, \Gamma_2 = \alpha\alpha\beta, \alpha\beta\beta$ ($\alpha \neq \beta$) and $F_1, F_2 = ffg, ffg$ ($f \neq g$). The constraint gives

$$\begin{aligned} & 3B_{\alpha\alpha\beta, \alpha\beta\beta}^{ffg, ffg} + (3-2)B_{\alpha\alpha\beta, \alpha\beta\beta}^{ffg, ffg} + B_{\alpha\alpha\alpha, \beta\beta\beta}^{fff, fgg} + (2-1)B_{\alpha\beta\beta, \alpha\alpha\beta}^{fgg, fff} \\ & = 4B_{\alpha\alpha\beta, \alpha\beta\beta}^{ffg, ffg} + B_{\alpha\alpha\alpha, \beta\beta\beta}^{fff, fgg} + B_{\alpha\beta\beta, \alpha\alpha\beta}^{fgg, fff} = 0, \end{aligned} \quad (4.91)$$

where minus signs in the first line come from the property that $B_{\Gamma_2, \Gamma_1}^{F_2, F_1} = -B_{\Gamma_1, \Gamma_2}^{F_1, F_2}$.

An immediate consequence of the identity is that the divergent part of the λ -dependent contributions, calculated from \mathbf{T}_1 in (4.64), must vanish, after the summation over the 9 different contributions from quark pairs on the different baryonic parts A, B is taken. The λ -dependent part of the contribution of quark contractions on the same baryonic parts is compensated by the quark field renormalization. Thus the renormalization of the bare 6-quark operator is λ -independent as expected from gauge invariance.

We thus need only to calculate the contributions from \mathbf{T}_0 , which can be classified into the following 4 different combinations for a pair of two indices:

$$\begin{pmatrix} f \\ \alpha \end{pmatrix} \begin{pmatrix} f \\ \alpha \end{pmatrix} \Rightarrow -(N+1) \begin{pmatrix} f \\ \alpha \end{pmatrix} \begin{pmatrix} f \\ \alpha \end{pmatrix}, \quad (4.92)$$

$$\begin{pmatrix} f \\ \alpha \end{pmatrix} \begin{pmatrix} f \\ \beta \end{pmatrix} \Rightarrow (1-2N) \begin{pmatrix} f \\ \alpha \end{pmatrix} \begin{pmatrix} f \\ \beta \end{pmatrix} + (N-2) \begin{pmatrix} f \\ \beta \end{pmatrix} \begin{pmatrix} f \\ \alpha \end{pmatrix}, \quad (4.93)$$

$$\begin{pmatrix} f_1 \\ \alpha \end{pmatrix} \begin{pmatrix} f_2 \\ \alpha \end{pmatrix} \Rightarrow - \begin{pmatrix} f_1 \\ \alpha \end{pmatrix} \begin{pmatrix} f_2 \\ \alpha \end{pmatrix} - N \begin{pmatrix} f_2 \\ \alpha \end{pmatrix} \begin{pmatrix} f_1 \\ \alpha \end{pmatrix}, \quad (4.94)$$

$$\begin{pmatrix} f_1 \\ \alpha \end{pmatrix} \begin{pmatrix} f_2 \\ \beta \end{pmatrix} \Rightarrow \left\{ \begin{pmatrix} f_1 \\ \alpha \end{pmatrix} \begin{pmatrix} f_2 \\ \beta \end{pmatrix} - 2 \begin{pmatrix} f_1 \\ \beta \end{pmatrix} \begin{pmatrix} f_2 \\ \alpha \end{pmatrix} \right\} + N \left\{ \begin{pmatrix} f_2 \\ \beta \end{pmatrix} \begin{pmatrix} f_1 \\ \alpha \end{pmatrix} - 2 \begin{pmatrix} f_2 \\ \alpha \end{pmatrix} \begin{pmatrix} f_1 \\ \beta \end{pmatrix} \right\}, \quad (4.95)$$

where $f \neq g$ and $\alpha \neq \beta \in (1, 2)$ (Right) or $\in (3, 4)$ (Left).

The computation can be made according to the following steps:

i.) Select the total flavor content e.g. $3f + 3g$ or $4f + 2g$ ($f \neq g$). These are the only cases for baryon operators with $N_f = 2$, but the approach is also applicable to more general cases ($N_f > 2$).

ii.) Given a flavor content classify all the possible sets of Dirac labels in the chiral basis e.g. 111223, 112234, ... It is obvious from the rules above that some have equivalent renormalization at 1-loop e.g. 111223 and 112223 with $1 \leftrightarrow 2$, and also those with hatted and unhatted indices exchanged e.g. 111223 and 133344.

iii.) For given flavor and Dirac sets generate all possible operators. Then generate all gauge identities between them and determine a maximally independent set $\{\mathcal{S}_i\}$.

iv.) Compute the divergent parts of the members of the independent basis:

$$\Gamma_i^{\text{div}} = \frac{1}{2\epsilon} \gamma_{ij} \mathcal{S}_j. \quad (4.96)$$

v.) Finally compute the eigenvalues and corresponding eigenvectors of γ^T to determine the operators which renormalize diagonally at 1-loop.

Some of the steps are quite tedious if carried out by hand. e.g. in the case $3f + 3g$ and Dirac indices 112234 there are initially 68 operators in step iii.) with 38 independent gauge identities, and hence an independent basis of 30 operators. However all the steps above can be easily implemented in an algebraic computer program using MATHEMATICA or MAPLE.

For $N_f = 2$ the quark $f(g)$ has $I_3 = 1/2$ ($-1/2$). If an eigenvalue is non-degenerate the corresponding eigenvector belongs to a certain representation of the isospin group. If the eigenvalue is degenerate then linear combinations of them belong to definite representations. For the $3f + 3g$ case they can have $I = 0, 1, 2, 3$. Eigenvectors with $I = 0, 2$ are odd under the interchange $f \leftrightarrow g$ and those with $I = 1, 3$ are even. The operators in the case $4f + 2g$ have $I_3 = 1$ and hence have $I = 1, 2, 3$. The eigenvectors in this case can be obtained from those of the $3f + 3g$ case by applying the isospin raising operator.

The complete list of eigenvalues and possible isospins are given in Tables 4.1-4.3. The most important results are summarized as follows.

1) For the $3f + 3g$ (and $4f + 2g$) cases all eigenvalues $\gamma_j \leq 48d = 2\gamma_N$, where γ_N is the 1-loop anomalous dimension of the nucleon (3-quark) operator.

2) It is easy to construct eigenvectors with eigenvalue $2\gamma_N$ e.g. operators of the form $B_{\alpha[\beta,\alpha]}^{ffg} B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ggf}$ since there is no contribution from diagrams where the gluon line joins quarks in the different baryonic parts.

3) Operators with higher isospin generally have smaller eigenvalues.

We now consider the renormalization of 6-quark operators which appear at the tree level of the OPE more explicitly. Since

$$C\gamma_5 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad (4.97)$$

in the chiral representation, the nucleon operator is written as

$$B_\alpha^f = B_{\alpha+\hat{\alpha},[2,1]}^{ffg} + B_{\alpha+\hat{\alpha},[\hat{2},\hat{1}]}^{ffg} \quad (4.98)$$

where $\alpha = 1, 2$, $\hat{\alpha} = \alpha + 2$, and $f \neq g$. This has anomalous dimension $\gamma_N = 24d$.

Two independent 6-quark operators occurring in the OPE at tree level can be decomposed as follows. The spin-singlet ($S = 0$) and isospin-triplet ($I = 1$) operator becomes

$$B_{\alpha+\hat{\alpha},[\beta,\alpha]+[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\beta+\hat{\beta},[\beta,\alpha]+[\hat{\beta},\hat{\alpha}]}^{ffg} = B_I^{01} + B_{II}^{01} + B_{III}^{01} + B_{IV}^{01} + B_V^{01} + B_{VI}^{01} \quad (4.99)$$

where ($\alpha \neq \beta$)

$$B_I^{01} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\beta[\beta,\alpha]}^{ffg} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\beta}[\hat{\beta},\hat{\alpha}]}^{ffg}, \quad (4.100)$$

$$B_{II}^{01} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\beta[\hat{\beta},\hat{\alpha}]}^{ffg} + B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\beta[\beta,\alpha]}^{ffg} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\beta[\beta,\alpha]}^{ffg} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\hat{\beta}[\hat{\beta},\hat{\alpha}]}^{ffg}, \quad (4.101)$$

$$B_{III}^{01} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\hat{\beta}[\beta,\alpha]}^{ffg} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\beta[\beta,\alpha]}^{ffg} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\beta[\hat{\beta},\hat{\alpha}]}^{ffg} + B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\beta}[\hat{\beta},\hat{\alpha}]}^{ffg}, \quad (4.102)$$

$$B_{IV}^{01} = B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\beta[\hat{\beta},\hat{\alpha}]}^{ffg} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\hat{\beta}[\beta,\alpha]}^{ffg}, \quad (4.103)$$

$$B_V^{01} = B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\beta}[\beta,\alpha]}^{ffg} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\beta[\hat{\beta},\hat{\alpha}]}^{ffg}, \quad (4.104)$$

$$B_{VI}^{01} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\hat{\beta}[\hat{\beta},\hat{\alpha}]}^{ffg} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\beta[\beta,\alpha]}^{ffg}. \quad (4.105)$$

In the above some contributions are obtained from interchanges under $(1, 2) \leftrightarrow (3, 4)$ or $(1, 3) \leftrightarrow (2, 4)$.

Similarly the spin-triplet ($S = 1$) and isospin-singlet ($I = 0$) operator is decomposed as

$$B_{\alpha+\hat{\alpha},[\beta,\alpha]+[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\alpha+\hat{\alpha},[\beta,\alpha]+[\hat{\beta},\hat{\alpha}]}^{ggf} = B_I^{10} + B_{II}^{10} + B_{III}^{10} + B_{IV}^{10} + B_V^{10} + B_{VI}^{10},$$

$$(4.106)$$

where

$$B_I^{10} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\alpha[\beta,\alpha]}^{ggf} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ggf}, \quad (4.107)$$

$$B_{II}^{10} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ggf} + B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\alpha[\beta,\alpha]}^{ggf} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\alpha}[\beta,\alpha]}^{ggf} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ggf}, \quad (4.108)$$

$$B_{III}^{10} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\hat{\alpha}[\beta,\alpha]}^{ggf} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\alpha[\beta,\alpha]}^{ggf} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ggf} + B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ggf}, \quad (4.109)$$

$$B_{IV}^{10} = B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ggf} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\hat{\alpha}[\beta,\alpha]}^{ggf}, \quad (4.110)$$

$$B_V^{10} = B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\hat{\alpha}[\beta,\alpha]}^{ggf} + B_{\hat{\alpha}[\beta,\alpha]}^{ffg} B_{\alpha[\hat{\beta},\hat{\alpha}]}^{ggf}, \quad (4.111)$$

$$B_{VI}^{10} = B_{\alpha[\beta,\alpha]}^{ffg} B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ggf} + B_{\hat{\alpha}[\hat{\beta},\hat{\alpha}]}^{ffg} B_{\alpha[\beta,\alpha]}^{ggf}. \quad (4.112)$$

It is important to note here that operators B_{VI}^{SI} for both cases ($SI = 01$ and 10) have the maximal anomalous dimension at 1-loop, since as noted in point 2) above, no 1-loop correction from \mathbf{T}_0 joining quarks from the two baryonic components exists for $B_{\alpha\beta\gamma,\hat{\alpha}'\hat{\beta}'\hat{\gamma}'}^{F_1,F_2}$ type of operators. Therefore there always exist some operators with $\beta_A = 0$ which dominate in the OPE at short distance.

The 1-loop corrections $\Gamma^{(1)}$ to 6-quark operators B^{SI} are summarized as:

$$\begin{aligned} (\Gamma_I^{01})^{(1)} &= -12\frac{d}{\epsilon}B_I^{01}, \quad (\Gamma_{II}^{01})^{(1)} = 12\frac{d}{\epsilon}B_{II}^{01}, \quad (\Gamma_{III}^{01})^{(1)} = 0, \\ (\Gamma_{IV}^{01})^{(1)} &= 0, \quad (\Gamma_V^{01})^{(1)} = 6\frac{d}{\epsilon}B_V^{01} + 6\frac{d}{\epsilon}B_{VI}^{01}, \quad (\Gamma_{VI}^{01})^{(1)} = 24\frac{d}{\epsilon}B_{VI}^{01}, \end{aligned} \quad (4.113)$$

for $SI = 01$. The last two results can be written as

$$(\Gamma_{V'}^{01})^{(1)} = 6\frac{d}{\epsilon}B_{V'}^{01}, \quad (\Gamma_{VI'}^{01})^{(1)} = 24\frac{d}{\epsilon}B_{VI'}^{01}, \quad (4.114)$$

where

$$B_{V'}^{01} = B_V^{01} - \frac{1}{3}B_{VI}^{01}, \quad B_{VI'}^{01} = B_{VI}^{01}. \quad (4.115)$$

Similarly for $SI = 10$

$$\begin{aligned} (\Gamma_I^{10})^{(1)} &= -4\frac{d}{\epsilon}B_I^{10}, \quad (\Gamma_{II}^{10})^{(1)} = 20\frac{d}{\epsilon}B_{II}^{10}, \quad (\Gamma_{III}^{10})^{(1)} = 0, \\ (\Gamma_{IV}^{10})^{(1)} &= 8\frac{d}{\epsilon}B_{IV}^{10}, \quad (\Gamma_{V'}^{10})^{(1)} = 6\frac{d}{\epsilon}B_{V'}^{10}, \quad (\Gamma_{VI'}^{10})^{(1)} = 24\frac{d}{\epsilon}B_{VI'}^{10}, \end{aligned} \quad (4.116)$$

where

$$B_{V'}^{10} = B_V^{10} - \frac{1}{3}B_{VI}^{10}, \quad B_{VI'}^{10} = B_{VI}^{10}. \quad (4.117)$$

Denoting the eigenvalues of the anomalous dimension matrix by γ_C , the values of γ^{SI} defined by

$$\gamma_C - 2\gamma_N = 2d\gamma^{SI}, \quad (4.118)$$

are given in table 4.4 ($N = 3$), which shows, in both cases, that the largest value is zero while others are all negative. The case 2 in sect. 4.1 is realized: $\beta_C = 0$ and

$$\beta_{C'} = \beta_0^{01} = -\frac{6}{33 - 2N_f} \quad \text{for } S = 0, I = 1, \quad (4.119)$$

$$\beta_{C'} = \beta_0^{10} = -\frac{2}{33 - 2N_f} \quad \text{for } S = 1, I = 0. \quad (4.120)$$

4.4 Short distance behavior of the potentials and the repulsive core

As discussed before, the NN potential at the leading order of the derivative expansion is given by

$$V^I(\mathbf{r}) = V_0^I(r) + V_\sigma^I(r)\vec{\sigma}_1 \cdot \vec{\sigma}_2 + V_T^I(r)S_{12} + O(\nabla). \quad (4.121)$$

From the result in the previous subsection, the OPE of NN at tree level can be written as

$$B_\alpha^f(x + y/2)B_\beta^g(x - y/2) \simeq c_{VI}B_{VI,\alpha\beta}^{fg}(x) + c_{II}(-\log r)^{\beta_0^{SI}}B_{II,\alpha\beta}^{fg}(x) + \dots \quad (4.122)$$

where c_{VI} and c_{II} are some constants, and \dots represents other contributions, which are less singular than the first two at short distance. The spinor and flavor indices α, β and f, g are explicitly written here. The anomalous dimensions β_0^{SI} are given in (4.119) and (4.120).

In the case that $S = 0$ and $I = 1$ ($\alpha \neq \beta$ and $f = g$ in eq.(4.122)), the leading contributions couple only to the $J = L = 0$ state given by

$$|E\rangle = |L_z = 0, S_z = 0, I_z = 1\rangle_{L=0, S=0, I=1} = |0, 0, 1\rangle_{0,0,1}. \quad (4.123)$$

The relevant matrix elements are

$$c_{VI}\langle 0|B_{VI,\alpha\beta}^{fg}|0, 0, 1\rangle_{0,0,0} = A_{VI}^0 Y_{00}[\alpha\beta]\{fg\}_1, \quad (4.124)$$

$$c_{II}\langle 0|B_{II,\alpha\beta}^{fg}|0, 0, 1\rangle_{0,0,0} = A_{II}^0 Y_{00}[\alpha\beta]\{fg\}_1, \quad (4.125)$$

where A_{II}^0 and A_{VI}^0 are non-perturbative constants, Y_{LL_z} is a spherical harmonic function, $[\alpha\beta] = (\delta_{\alpha 1}\delta_{\beta 2} - \delta_{\beta 1}\delta_{\alpha 2})/\sqrt{2}$ represents the $(S, S_z) = (0, 0)$ component, and $\{fg\}_1 = \delta_{f1}\delta_{g1}$ corresponds to isospin $(I, I_z) = (1, 1)$. The wave function at short distance is dominated by

$$\varphi_E^{1S_0}(y) = \langle 0|B_\alpha^f(x + y/2)B_\beta^g(x - y/2)|0, 0, 1\rangle_{0,0,1}$$

$$\simeq \left(A_{VI}^0 + A_{II}^0 (-\log r)^{\beta_0^{01}} \right) \phi(^1S_0, 0)^{11} + \dots, \quad (4.126)$$

where $\phi(^1S_0, J_z = 0)^{II_z=11} = Y_{00}[\alpha\beta]\{fg\}_1$. This wave function leads to

$$\frac{\nabla^2}{2m} \varphi_E^{^1S_0}(y) \simeq \frac{(-\log r)^{\beta_0^{01}-1}}{r^2} \frac{-\beta_0^{01} A_{II}^0}{m_N} \phi(^1S_0, 0)^{11} + \dots \quad (4.127)$$

where $m = m_N/2$ is the reduced mass of the two nucleon system. Since S_{12} is zero on $\phi(^1S_0, 0)^{11}$, we have

$$V_c^{01}(r) \varphi_E^{^1S_0}(y) \simeq \frac{(-\log r)^{\beta_0^{01}-1}}{r^2} \frac{-\beta_0^{01} A_{II}^0}{m_N} \phi(^1S_0, 0)^{11} + \dots \quad (4.128)$$

where $V_c^{01}(r) = V_0(r) - 3V_\sigma(r)$. Therefore the potential is obtained as

$$V_c^{01}(r) \simeq F^{01}(r) \frac{A_{II}^0}{A_{VI}^0}. \quad (4.129)$$

where

$$F^{SI}(r) = \frac{-\beta_0^{SI} (-\log r)^{\beta_0^{SI}-1}}{m_N r^2}. \quad (4.130)$$

The potential diverges as $F^{01}(r)$ in the $r \rightarrow 0$ limit, which is a little weaker than r^{-2} .

In the case of the spin-triplet and isospin-singlet state ($S = 1$ and $I = 0$), the leading contributions in eq.(4.122) couple only to the $J = 1$ state, which is given by

$$|E\rangle = |^3S_1, J_z = 1\rangle + x|^3D_1, J_z = 1\rangle, \quad (4.131)$$

where

$$|^3S_1, J_z = 1\rangle = |L_z = 0, S_z = 1\rangle_{L=0, S=1}, \quad (4.132)$$

$$|^3D_1, J_z = 1\rangle = \frac{1}{\sqrt{10}} \left[|0, 1\rangle - \sqrt{3}|1, 0\rangle + \sqrt{6}|2, -1\rangle \right]_{L=2, S=1}, \quad (4.133)$$

x is the mixing coefficient, which is determined by QCD dynamics, and $^{2S+1}L_J$ specifies quantum numbers of the state. We here drop indices I and I_z unless necessary.

Relevant matrix elements are given by

$$c_i \left\langle 0 \left| B_{i, \alpha\beta}^{fg} \right| ^3S_1, 1 \right\rangle = B_i^0 \phi(^3S_1), \quad c_i \left\langle 0 \left| B_{i, \alpha\beta}^{fg} \right| ^3D_1, 1 \right\rangle = 0, \quad (4.134)$$

for $i = II$ and VI , where B_i^0 are non-perturbative constants, and

$$\phi(^3S_1) = Y_{00}(\theta, \phi) \{\alpha\beta\}_1 [fg], \quad (4.135)$$

with $\{\alpha\beta\}_1 = \delta_{\alpha 1} \delta_{\beta 1}$.

Using the above results, the BS wave function becomes

$$\varphi_E^{J=1}(y) \simeq \left\{ B_{VI}^0 + (-\log r)^{\beta_0^{10}} B_{II}^0 \right\} \phi({}^3S_1), \quad (4.136)$$

which leads to

$$\frac{\nabla^2}{2m} \varphi_E^{J=1}(y) \simeq \frac{-\beta^{10}}{m_N} \frac{(-\log r)^{\beta_0^{10}-1}}{r^2} B_{II}^0 \phi({}^3S_1). \quad (4.137)$$

On the other hand,

$$V(y) \varphi_E^{J=1}(y) \simeq B_{VI}^0 V_c^{10}(r) \phi({}^3S_1) + 2\sqrt{2} V_T(r) B_{VI}^0 \phi({}^3D_1), \quad (4.138)$$

where $V_c^{10}(r) = V_0^0(r) + V_\sigma^0(r)$ and

$$\phi({}^3D_1) = \frac{1}{\sqrt{10}} \left[Y_{20} \{\alpha\beta\}_1 - \sqrt{3} Y_{21} \{\alpha\beta\}_0 + \sqrt{6} Y_{22} \{\alpha\beta\}_{-1} \right] [fg], \quad (4.139)$$

with $\{\alpha\beta\}_{-1} = \delta_{\alpha 2} \delta_{\beta 2}$ and $\{\alpha\beta\}_0 = (\delta_{\alpha 1} \delta_{\beta 2} + \delta_{\beta 1} \delta_{\alpha 2})/\sqrt{2}$.

By comparing eq.(4.137) with eq.(4.138), we obtain

$$V_c^{10}(r) \simeq F^{10}(r) \frac{B_{II}^0}{B_{VI}^0}, \quad V_T(r) \simeq 0. \quad (4.140)$$

This shows that the central potential $V_c^{10}(r)$ diverges as $F^{10}(r)$ in the $r \rightarrow 0$ limit, which is a little weaker than $1/r^2$, while the tensor potential $V_T(r)$ becomes zero in this limit at the tree level in the OPE.

While the OPE predicts the functional form of the central potentials at short distance for both $S = 0$ and $S = 1$ channels, it can not determine whether it is repulsive or attractive. The NN operators are decomposed as

$$B_\alpha^f B_\beta^g = [B_I + B_{II} + B_{III} + B_{IV} + B_V + B_{VI}]_{\alpha\beta}^{fg}, \quad (4.141)$$

where

$$(B_I)_{\alpha\beta}^{fg} = [B_{RR} B_{RR} + B_{LL} B_{LL}]_{\alpha\beta}^{fg}, \quad (4.142)$$

$$(B_{II})_{\alpha\beta}^{fg} = [B_{RR} B_{RL} + B_{RL} B_{RR} + B_{LL} B_{LR} + B_{LR} B_{LL}]_{\alpha\beta}^{fg}, \quad (4.143)$$

$$(B_{III})_{\alpha\beta}^{fg} = [B_{RR} B_{LR} + B_{LR} B_{RR} + B_{LL} B_{RL} + B_{RL} B_{LL}]_{\alpha\beta}^{fg}, \quad (4.144)$$

$$(B_{IV})_{\alpha\beta}^{fg} = [B_{RL} B_{RL} + B_{LR} B_{LR}]_{\alpha\beta}^{fg}, \quad (4.145)$$

$$(B_V)_{\alpha\beta}^{fg} = [B_{RL} B_{LR} + B_{LR} B_{RL}]_{\alpha\beta}^{fg}, \quad (4.146)$$

$$(B_{VI})_{\alpha\beta}^{fg} = [B_{RR} B_{LL} + B_{LL} B_{RR}]_{\alpha\beta}^{fg}. \quad (4.147)$$

Here 3-quark operators in terms of left- and right- handed component are defined by

$$B_{AX,\alpha}^f = (P_A)_{\alpha\beta} B_{X,\beta}^f, \quad B_{X,\alpha}^f = B_{\alpha\beta\gamma}^{fgh} (C\gamma_5 P_X)_{\beta\gamma} (i\tau_2)_{gh}, \quad (4.148)$$

for $A, X = R$ or L . We need to know

$$\langle 0 | (B_i)_{\alpha\beta}^{fg} | 2N, E \rangle \quad (4.149)$$

for $i = II, VI$.

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For $f \neq g$, Lorentz covariance leads to

$$\langle 0 | B_X^f B_Y^g | 2N, E \rangle = \sum_{A,B=R,L} C_{XY}^{AB}(s) P_A u(\mathbf{p}, \sigma_1) P_B u(-\mathbf{p}, \sigma_2), \quad (4.150)$$

where $s = E^2 = 4(\mathbf{p}^2 + m_N^2)$ with the total energy E in the center of mass frame, σ_i ($i = 1, 2$) is the spin of the i -th nucleon, and C_{XY}^{AB} is an unknown function of s . Note that spinor indices are suppressed here. Invariance of QCD under the parity transformation $P B_X P^{-1} = \gamma_4 B_{\bar{X}}$ where $\bar{R} = L$ and $\bar{L} = R$ gives

$$\begin{aligned} (4.150) &= \langle 0 | P B_X^f B_Y^g P^{-1} P | 2N, E \rangle = \sum_{A,B} C_{\bar{X}\bar{Y}}^{AB} P_A \gamma_4 u(-\mathbf{p}, \sigma_1) P_{\bar{B}} \gamma_4 u(\mathbf{p}, \sigma_2) \\ &= \sum_{A,B} C_{\bar{X}\bar{Y}}^{\bar{A}\bar{B}} P_A u(\mathbf{p}, \sigma_1) P_B u(-\mathbf{p}, \sigma_2), \end{aligned} \quad (4.151)$$

where $\gamma_4 u(-\mathbf{p}, \sigma_1) = u(\mathbf{p}, \sigma_1)$ is used. The above relation implies $C_{\bar{X}\bar{Y}}^{\bar{A}\bar{B}} = C_{XY}^{AB}$. Therefore the matrix elements are evaluated as

$$\langle 0 | (B_{II})_{\alpha\beta}^{fg\pm gf} | 2N, E \rangle = C_{RL+LR}^{RR,\pm} \{ (P_R \otimes P_R + P_L \otimes P_L) u(\mathbf{p}, \sigma_1) u(-\mathbf{p}, \sigma_2) \}_{\alpha\beta \mp \beta\alpha} \quad (4.152)$$

and

$$\langle 0 | (B_{VI})_{\alpha\beta}^{fg\pm gf} | 2N, E \rangle = C_{RL}^{RL,\pm} \{ (P_R \otimes P_L + P_L \otimes P_R) u(\mathbf{p}, \sigma_1) u(-\mathbf{p}, \sigma_2) \}_{\alpha\beta \mp \beta\alpha} \quad (4.153)$$

The spinor in Dirac representation for γ matrices (Itzykson and Zuber, 1980) is given by

$$u(\pm\mathbf{p}, +) = \frac{1}{\sqrt{E_N + m_N}} \begin{pmatrix} E_N + m_N \\ 0 \\ \mp p_z \\ 0 \end{pmatrix}, \quad u(\pm\mathbf{p}, -) = \frac{1}{\sqrt{E_N + m_N}} \begin{pmatrix} 0 \\ E_N + m_N \\ 0 \\ \pm p_z \end{pmatrix} \quad (4.154)$$

for $\mathbf{p} = (0, 0, p_z > 0)$, where $E_N = \sqrt{\mathbf{p}^2 + m_N^2}$. For $I = 1$ ($fg + gf$) and $S = 0$ ($\sigma_1 = +$ and $\sigma_2 = -$) the above explicit form for the spinors gives

$$\{ (P_R \otimes P_R + P_L \otimes P_L) u(\mathbf{p}, +) u(-\mathbf{p}, -) \}_{12-21} = E_N, \quad (4.155)$$

$$\{ (P_R \otimes P_L + P_L \otimes P_R) u(\mathbf{p}, +) u(-\mathbf{p}, -) \}_{12-21} = m_N, \quad (4.156)$$

while, for $I = 0$ ($fg - gf$) and $S = 1$ ($\sigma_1 = +$ and $\sigma_2 = +$)

$$\{ (P_R \otimes P_R + P_L \otimes P_L) u(\mathbf{p}, +) u(-\mathbf{p}, +) \}_{11} = m_N, \quad (4.157)$$

$$\{(P_R \otimes P_L + P_L \otimes P_R)u(\mathbf{p}, +)u(-\mathbf{p}, +)\}_{11} = E_N. \quad (4.158)$$

Finally the ratio of the matrix elements becomes

$$\frac{\langle 0|(B_{II})_{12}^{fg+gf}|2N, E\rangle}{\langle 0|(B_{VI})_{12}^{fg+gf}|2N, E\rangle} = \frac{E_N}{m_N} \frac{C_{RL+LR}^{RR,+}(s)}{C_{RL}^{RL,+}(s)} \quad (4.159)$$

for $fg + gf$ and $(\sigma_1, \sigma_2) = (+, -)$ (1S_0), and

$$\frac{\langle 0|(B_{II})_{11}^{fg-gf}|2N, E\rangle}{\langle 0|(B_{VI})_{11}^{fg-gf}|2N, E\rangle} = \frac{m_N}{E_N} \frac{C_{RL+LR}^{RR,-}(s)}{C_{RL}^{RL,-}(s)} \quad (4.160)$$

for $fg - gf$ and $(\sigma_1, \sigma_2) = (+, +)$ (3S_1), where $s = 4E_N^2$.

Unfortunately, the sign of the ratio for these matrix elements can not be determined. As a very crude estimation, the non-relativistic expansion for constituent quarks whose mass m_Q is given by $m_Q = m_N/3$ is considered. In the large m_Q limit, $\gamma_4 q_0 = q_0$ and $\gamma_4 u_0 = u_0$, where a subscript 0 for q and u means the 0-th order in the non-relativistic expansion. In this limit, it is easy to show $C_{XY}^{AB} = C$ for all X, Y, A, B , so that $C_{RL+LR}^{RR} = 2C$ and $C_{RL}^{RL} = C$. Furthermore the first order correction to $C_{XY}^{AB} = C$ vanishes in the expansion. Therefore the leading order of the non-relativistic expansion gives

$$\frac{\langle 0|(B_{II})_{12}^{fg+gf}|2N, E\rangle}{\langle 0|(B_{VI})_{12}^{fg+gf}|2N, E\rangle} \simeq 2 + \mathcal{O}\left(\frac{\mathbf{p}^2}{m_Q^2}\right) \quad (4.161)$$

for $(\sigma_1, \sigma_2) = (+, -)$ (1S_0), and

$$\frac{\langle 0|(B_{II})_{11}^{fg-gf}|2N, E\rangle}{\langle 0|(B_{VI})_{11}^{fg-gf}|2N, E\rangle} \simeq 2 + \mathcal{O}\left(\frac{\mathbf{p}^2}{m_Q^2}\right) \quad (4.162)$$

for $(\sigma_1, \sigma_2) = (+, +)$ (3S_1). For both cases, the ration has positive sign, which gives repulsion at short distance, the repulsive core.

Table 4.1 Eigenvalues γ_j of the anomalous dimension matrix γ and isospins of the corresponding eigenvectors for the case $3\bar{f}3g$.

Dirac indices	$\gamma_j/(2d)$	I
111111	-24	0
111112	-24	0, 1
111122	-4	0
	-24	0, 1
	-40	2
111222	-4	0
	-12	1
	-24	0, 1
	-40	2
	-72	3
111113	-16	0, 1
111123	-6	0, 1
	-16	0, 1
	-24	1, 2
111223	0	0, 1
	-6	0, 1
	-16	0, 1
	-18	1, 2
	-24	1, 2
	-48	2, 3
111133	-4	0
	-16	0, 1, 2
111134	0	1
	-4	0
	-12	1
	-16	0, 1, 2
111233	4	1
	-4	0
	-8	0, 1, 1
	-16	0, 1, 2
	-32	1, 2, 3

Table 4.2 As in Table4.1 (continued).

Dirac indices	$\gamma_j/(2d)$	I
111234	20	0
	8	1
	4	1
	0	1
	-4	0
	-8	0, 1, 1, 2
	-12	1
	-16	0, 0, 0, 1, 1, 2, 2, 2
	-32	1, 2, 3
112233	8	0
	4	1
	-4	0, 0, 1, 2
	-8	0, 1, 1, 2
	-16	0, 1, 2
	-28	2
	-30	1, 2, 3
112234	20	0
	12	1
	8	0, 1
	4	1
	0	1, 1
	-4	0, 0, 1, 2
	-8	0, 1, 1, 2
	-12	1
	-16	0, 0, 1, 1, 2, 2, 2
	-28	2
	-32	1, 2, 3
	-36	1, 2, 3
111333	-6	0, 1
	-24	0, 1, 2, 3
111334	0	0, 1, 1, 2
	-6	0, 1
	-18	1, 2
	-24	0, 1, 2, 3

Table 4.3 As in Table4.1 (continued).

Dirac indices	$\gamma_j/(2d)$	I
112334	24	0, 1
	6	0, 1
	0	0, 0, 1, 1, 1, 1, 2, 2
	-6	0, 1
	-12	1, 1, 2, 2
	-18	1, 1, 2, 2
	-24	0, 1, 2, 3
	-30	0, 1, 2, 3

Table 4.4 The value of γ^{SI} (defined in (4.72)) for each eigen operator in the $SI = 01$ and $SI = 10$ states.

	I	II	III	IV	V'	VI'
γ^{01}	-36	-12	-24	-24	-18	0
γ^{10}	-28	-4	-24	-16	-18	0

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Concluding Remarks

In this lecture, we consider two different but closely related topics in lattice QCD approaches to hadron interactions.

In the first part, we explain the Lüscher's formula, which relates the scattering phase shift to the two particle energy in the finite volume. Although this formula is well-established and has appeared in the well-written reference (Lüscher, 1991), a comprehensive (but less rigorous) derivation for the formula has been attempted in this lecture for the $\pi\pi$ system as an example with the emphasis on the BS wave function. It is important to stress that the BS wave function at large separation behaves as the free scattering wave with the phase shift which is determined by the unitarity of the S -matrix in QCD. The Lüscher's formula can be obtained from this asymptotic behavior of the BS wave function.

In the second part, on the other hand, we consider the BS wave function at non-asymptotic region where the interaction between two particles exists, in order to define the potential in quantum field theories. We apply this method for the two nucleons to calculate the NN potential in QCD. The first result from lattice QCD has a good shape, which reproduces both the repulsive core at short distance and the attractive well at medium and long distances.

In the last part, the origin of the repulsive core is theoretically investigated by the OPE and the renormalization group. The analysis predicts the r dependence of the potentials at short distance, though it can not tell the sign of the potential, positive (repulsive) or negative (attractive). A crude estimate by the non-relativistic quark gives the positive sign, the repulsive core.

The method to investigate potentials through the BS wave function in lattice QCD is a quite new approach, which may be applied to the following directions.

(1) In order to extract the realistic NN potentials from lattice QCD, it is necessary to carry out full QCD simulations near the physical u , d quark masses. Studies along this line using 2+1-flavor QCD configuration generated by PACS-CS Collaboration (Aoki *et al.*, 2009a) is currently under way (Ishii *et al.*, 2008).

(2) The hyperon-nucleon (YN) and hyperon-hyperon (YY) potentials are essential to understand properties of hyper nuclei and the hyperonic matter inside the neutron star. While experimental scattering data are very limited due to the short life-time of hyperons, the NN , YN and YY interactions on the lattice can be investigated in the same manner just by changing only the quark flavors. The ΞN potential in quenched QCD (Nemura *et al.*, 2009) and the ΛN potential in both quenched and full QCD (Nemura *et al.*, 2008) are examined as a first step toward the systematic understanding of baryonic potentials. To this connection, the OPE analysis should be

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extended to the $N_f = 3$ case, in order to reveal the nature of the repulsive core in baryon-baryon potentials. Since quark mass terms can be neglected in the OPE at short distance, the analysis can be done in the exact $SU(3)$ symmetric limit.

(3) The three-nucleon force is thought to play important roles in nuclear structures and in the equation of state in high density matter. Since the experimental information is very limited, the extension of the method to the three nucleons may lead to the first principle extractions of the three-nucleon potentials in QCD. It is also interesting to investigate the existence or the absence of the repulsive core in the three-nucleon potentials. The calculation of anomalous dimensions of 9-quark operators will be required at 2-loop level.

(4) More precise evaluations including numerical simulations of matrix elements $\langle 0|O_X|E\rangle$ will be needed to understand the nature of the core in the potential through the OPE analysis.

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